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(54) Title: METHOD OF IDENTIFYING INHIBITORS OF TIE-2

(57) Abstract: The present invention relates to polypeptides which comprise the ligand binding domain of Tie-2, crystalline forms of these polypeptides and the use of these crystalline forms to determine the three dimensional structure of the catalytic domain of Tie-2. The invention also relates to the use of the three dimensional structure of the Tie-2 catalytic domain both alone, or in complex with inhibitors, in methods of designing and/or identifying potential inhibitors of Tie-2 activity, for example, compounds which inhibit the binding of a native substrate to the Tie-2 catalytic domain.



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METHOD OF IDENTIFYING INHIBITORS OF TIE-2

RELATED APPLICATION

This application claims the benefit of U.S. Provisional Application No.
5 60/192,920, filed on March 29, 2000. The entire teachings of the above application is incorporated herein by reference.

BACKGROUND OF THE INVENTION

Angiogenesis is a fundamental process by which new blood vessels are formed
10 through sprouting, branching, proliferation, and tubule formation by endothelial cells from existing vasculature. In healthy humans, this neovascularization is under stringent control, normally occurring only during embryonic development, endometrial regulation, breast lactation and wound repair. However, in many pathological conditions, such as rheumatoid arthritis, solid tumors, Kaposi's sarcoma,
15 blindness due to ocular neovascularization, psoriasis and atherosclerosis, disease progression is dependent upon persistent angiogenesis. The vasculature, which is the conduit for drug delivery, is one of the most accessible tissues in the body. Each endothelial cell of tumor vessels is estimated to support 100 to 1,000 neighboring cells, yet in the absence of an angiogenic stimulus endothelial cells typically divide
20 only once every thousand days.

A number of polypeptide growth factors and their associated endothelial cell specific receptors have been discovered which are primarily responsible for the stimulation of endothelial cell growth, differentiation and the establishment of new vasculature. These growth factor receptors include the vascular endothelial growth
25 factor receptors (VEGFR) Flk-1 (mouse), KDR/VEG-FR-2 (human), Flt-1/VEGFR-1, and Flt-4/VEGFR-3. Receptors which are responsible for neovascularization also include the receptor tyrosine kinases Tie-1 and Tie-2.

Due to its role in regulating new vascular development, Tie-2 is a potential target for therapies aimed at controlling diseases which depend upon persistent
30 angiogenesis. The development of biochemical assays for Tie-2 has enabled drug

discovery to proceed along the pathways of identifying lead Tie-2 inhibitors by high-throughput screening of compound libraries and by testing compounds that mimic substrate structure; however, rational, structure-based design has not been possible up to this point because of the lack of accurate three-dimensional structural data for Tie-2
5 receptors.

SUMMARY OF THE INVENTION

The present invention relates to a polypeptide which comprises the catalytic domain of Tie-2, a crystalline form of this polypeptide and the use of structural
10 information derived from the crystalline form of the polypeptide for designing and/or identifying potential inhibitors of the binding of one or more native ligands to the catalytic domain of Tie-2.

In one embodiment, the present invention relates to a polypeptide comprising the catalytic domain of TIE-2 and having the amino acid sequence set forth in SEQ ID
15 NO: 2. In another embodiment, the invention relates to a crystalline form of this polypeptide or the polypeptide complexed with a ligand.

In another embodiment, the invention provides a method of determining the three dimensional structure of a crystalline polypeptide comprising the Tie-2 catalytic domain. In one embodiment, the method comprises the steps of (1) obtaining a crystal
20 of the polypeptide comprising the catalytic domain of Tie-2; (2) obtaining x-ray diffraction data for said crystal; and (3) solving the crystal structure of said crystal. The method optionally comprises the additional step of obtaining the polypeptide, with the three dimensional structure to be determined, prior to obtaining the crystal of said peptide.

25 In another embodiment, the method comprises the steps of (1) obtaining a crystal of the polypeptide comprising the catalytic domain of Tie-2; (2) obtaining x-ray diffraction data for said crystal; and (3) solving the crystal structure of said crystal by using said x-ray diffraction data and the atomic coordinates for the Tie-2 catalytic domain of a second polypeptide. The method optionally comprises the additional step
30 of obtaining the polypeptide, with the three dimensional structure to be determined, prior to obtaining the crystal of said peptide.

The invention further relates to a method for identifying a compound which inhibits the catalytic activity of Tie-2 by, for example, inhibiting the binding of natural substrates such as a tyrosyl polypeptide or protein or ATP, to the catalytic domain of Tie-2. Such a compound is referred to herein as a "Tie-2 inhibitor". The method
5 comprises the steps of (1) using a three-dimensional structure of Tie-2 as defined by the atomic coordinates of the catalytic domain of Tie-2; (2) employing the three dimensional structure to design or select a potential inhibitor; and (3) assessing the ability of the selected compound to inhibit the catalytic activity of Tie-2. The method can also include the step of providing the compound designed or selected in step 2, for
10 example, by synthesizing the compound or obtaining the compound from a compound library. In addition, the method can include the step of assessing the ability of the identified compound to bind to the catalytic domain of Tie-2 and/or assessing the ability of the identified compound to inhibit the binding of a natural ligand of Tie-2.

In another embodiment, the method for identifying a compound which inhibits
15 the catalytic activity of Tie-2, comprises the step of determining the ability of one or more functional groups and/or moieties of the compound, when present in, or bound to, the Tie-2 catalytic domain, to interact with one or more subsites of the Tie-2 catalytic domain. Generally, the Tie-2 catalytic domain is defined by the conserved homologous sequences when compared to other known tyrosine kinases. If the
20 compound is able to interact with a preselected number or set of subsites, or has a calculated interaction energy within a desired or preselected range, the compound is identified as a potential inhibitor of Tie-2.

The invention further provides a method of designing a compound which is a potential inhibitor of the catalytic activity of Tie-2. The method includes the steps of
25 (1) identifying one or more functional groups capable of interacting with one or more subsites of the Tie-2 catalytic domain; and (2) identifying a scaffold which presents the functional group, or functional groups, identified in step 1 in a suitable orientation for interacting with one or more subsites of the Tie-2 catalytic domain. The compound which results from attachment of the identified functional groups or
30 moieties to the identified scaffold is a potential inhibitor of Tie-2. The Tie-2 catalytic

domain is, generally, defined by the atomic coordinates of a polypeptide comprising the Tie-2 catalytic domain.

In yet another embodiment, the invention provides compounds which inhibit the catalytic activity of Tie-2 and which fit, or bind to, the Tie-2 catalytic domain.

5 Such compounds typically comprise one or more functional groups which, when the compound is bound in the Tie-2 catalytic domain, interact with one or more subsites of the catalytic domain. Generally, the Tie-2 catalytic domain is defined by the conserved homologous sequence when compared to other known tyrosine kinases. In a particular embodiment, the Tie-2 inhibitor is a compound which is identified or
10 designed by a method of the present invention.

The present invention further provides a method for treating a condition mediated by Tie-2 in a patient. The method comprises administering to the patient a therapeutically or prophylactically effective amount of a compound which inhibits the catalytic activity of Tie-2, such as a Tie-2 inhibitor of the invention, for example, a
15 compound identified as a Tie-2 inhibitor or designed to inhibit Tie-2 by a method of the present invention.

The present invention provides several advantages. For example, the invention provides the first detailed three dimensional structures of the ligand binding domain of a Tie-2 protein. The methods described herein can be used to facilitate
20 formation of Tie-2 crystals which diffract at high resolution. These structures enable the rational development of inhibitors of Tie-2 by permitting the design and/or identification of molecular structures having features which facilitate binding to the Tie-2 binding domain. The methods of use of the structures disclosed herein, thus, permit more rapid discovery of compounds which are potentially useful for the
25 treatment of conditions which are mediated, at least in part, by Tie-2 activity.

BRIEF DESCRIPTION OF THE DRAWINGS

Fig. 1 presents the amino acid sequence of human Tie-2 (SEQ ID NO: 1).

Fig. 2 presents the amino acid sequence which includes the catalytic domain of
30 human Tie-2 from amino acid 802 to amino acid 1124, and has a catalytically inactive point mutation at amino acid 964 (SEQ ID NO: 2).

Fig. 3A-3OO present the atomic coordinates for SEQ ID NO 2/inhibitor I complex.

Fig. 4A-4OO present the atomic coordinates for SEQ ID NO 2/inhibitor II complex.

5 Fig. 5A-5RR present the atomic coordinates for SEQ ID NO 2/inhibitor III complex.

Fig. 6A-6NN present the atomic coordinates for SEQ ID NO 2/inhibitor IV complex.

Fig. 7 shows the structure of a prototypical kinase, insulin receptor kinase.

10 Fig. 8 shows identifies regions of a pyrrolopyrimidine inhibitor (i.e., inhibitor I) which interact with the catalytic domain of Tie-2.

Fig. 9 shows a model of the catalytic domain of Tie-2 bound to inhibitor I. Subsites are shown in different colors.

15 DETAILED DESCRIPTION OF THE INVENTION

The present invention relates to the x-ray crystallographic study of polypeptides comprising the catalytic domain of Tie-2. The atomic coordinates which result from this study are of use in identifying compounds which fit in the catalytic domain and are, therefore, potential inhibitors of Tie-2. These Tie-2 inhibitors are of
20 use in methods of treating a patient having a condition which is modulated by or dependent upon Tie-2 activity, for example, a condition dependent on persistent angiogenesis.

There are at least 400 enzymes identified as protein kinases. These enzymes catalyze the phosphorylation of target protein substrates. The phosphorylation is
25 usually a transfer reaction of a phosphate group from ATP to the protein substrate. The specific structure in the target substrate to which the phosphate is transferred is a tyrosine, serine or threonine residue. Since these amino acid residues are the target structures for the phosphoryl transfer, these protein kinase enzymes are commonly referred to as tyrosine kinases or serine/threonine kinases.

30 The phosphorylation reactions, and counteracting phosphatase reactions, at the tyrosine, serine and threonine residues are involved in countless cellular processes that

underlie responses to diverse intracellular signals (typically mediated through cellular receptors), regulation of cellular functions, and activation or deactivation of cellular processes. A cascade of protein kinases often participate in intracellular signal transduction and are necessary for the realization of these cellular processes. Because
5 of their ubiquity in these processes, the protein kinases can be found as an integral part of the plasma membrane or as cytoplasmic enzymes or localized in the nucleus, often as components of enzyme complexes. In many instances, these protein kinases are an essential element of enzyme and structural protein complexes that determine where and when a cellular process occurs within a cell.

10 *Protein Tyrosine Kinases.* Protein tyrosine kinases (PTKs) are enzymes which catalyse the phosphorylation of specific tyrosine residues in cellular proteins. This post-translational modification of these substrate proteins, often enzymes themselves, acts as a molecular switch regulating cell proliferation, activation or differentiation (for review, see Schlessinger and Ulrich, 1992, *Neuron* 9:383-391). Aberrant or
15 excessive PTK activity has been observed in many disease states including benign and malignant proliferative disorders as well as diseases resulting from inappropriate activation of the immune system (e.g., autoimmune disorders), allograft rejection, and graft vs. host disease. In addition, endothelial-cell specific receptor PTKs such as KDR and Tie-2 mediate the angiogenic process, and are thus involved in supporting
20 the progression of cancers and other diseases involving inappropriate vascularization (e.g., diabetic retinopathy, choroidal neovascularization due to age-related macular degeneration, psoriasis, rheumatoid arthritis, retinopathy of prematurity, infantile hemangiomas, psoriasis and atherosclerosis.

Tyrosine kinases can be of the receptor-type (having extracellular,
25 transmembrane and intracellular domains) or the non-receptor type (being wholly intracellular).

Receptor Tyrosine Kinases (RTKs). The RTKs comprise a large family of transmembrane receptors with diverse biological activities. At present, at least nineteen (19) distinct RTK subfamilies have been identified. The receptor tyrosine
30 kinase (RTK) family includes receptors that are crucial for the growth and differentiation of a variety of cell types (Yarden and Ullrich, *Ann. Rev. Biochem.*

57:433-478, 1988; Ullrich and Schlessinger, *Cell* 61:243-254, 1990). The intrinsic function of RTKs is activated upon ligand binding, which results in phosphorylation of the receptor and multiple cellular substrates, and subsequently in a variety of cellular responses (Ullrich & Schlessinger, 1990, *Cell* 61:203-212). Thus, receptor
5 tyrosine kinase mediated signal transduction is initiated by extracellular interaction with a specific growth factor (ligand), typically followed by receptor dimerization, stimulation of the intrinsic protein tyrosine kinase activity and receptor trans-phosphorylation. Binding sites are thereby created for intracellular signal transduction molecules and lead to the formation of complexes with a spectrum of cytoplasmic
10 signaling molecules that facilitate the appropriate cellular response. (e.g., cell division, differentiation, metabolic effects, changes in the extracellular microenvironment) see Schlessinger and Ullrich, 1992, *Neuron* 9:1-20.

Proteins with SH2 (src homology -2) or phosphotyrosine binding (PTB) domains bind activated tyrosine kinase receptors and their substrates with high affinity
15 to propagate signals into cell. Both of the domains recognize phosphotyrosine. (Fantl *et al.*, 1992, *Cell* 69:413-423; Songyang *et al.*, 1994, *Mol. Cell. Biol.* 14:2777-2785; Songyang *et al.*, 1993, *Cell* 72:767-778; and Koch *et al.*, 1991, *Science* 252:668-678; Shoelson, *Curr. Opin. Chem. Biol.* (1997), 1(2), 227-234; Cowburn, *Curr. Opin. Struct. Biol.* (1997), 7(6), 835-838). Several intracellular substrate proteins that
20 associate with receptor tyrosine kinases (RTKs) have been identified. They may be divided into two principal groups: (1) substrates which have a catalytic domain; and (2) substrates which lack such a domain but serve as adapters and associate with catalytically active molecules (Songyang *et al.*, 1993, *Cell* 72:767-778). The specificity of the interactions between receptors or proteins and SH2 or PTB domains
25 of their substrates is determined by the amino acid residues immediately surrounding the phosphorylated tyrosine residue. For example, differences in the binding affinities between SH2 domains and the amino acid sequences surrounding the phosphotyrosine residues on particular receptors correlate with the observed differences in their substrate phosphorylation profiles (Songyang *et al.*, 1993, *Cell* 72:767-778).
30 Observations suggest that the function of each receptor tyrosine kinase is determined not only by its pattern of expression and ligand availability but also by the array of

downstream signal transduction pathways that are activated by a particular receptor as well as the timing and duration of those stimuli. Thus, phosphorylation provides an important regulatory step which determines the selectivity of signaling pathways recruited by specific growth factor receptors, as well as differentiation factor
5 receptors.

Several receptor tyrosine kinases such as FGFR-1, PDGFR, TIE-2 and c-Met, and growth factors that bind thereto, have been suggested to play a role in angiogenesis, although some may promote angiogenesis indirectly (Mustonen and Alitalo, *J. Cell Biol.* 129:895-898, 1995).

10 Tie-2 (TEK) is a member of a recently discovered family of endothelial cell specific receptor tyrosine kinases which is involved in critical angiogenic processes, such as vessel branching, sprouting, remodeling, maturation and stability. Tie-2 is the first mammalian receptor tyrosine kinase for which both agonist ligand(s) (e.g., Angiopoietin1 ("Ang1"), which stimulates receptor autophosphorylation and signal
15 transduction), and antagonist ligand(s) (e.g., Angiopoietin2 ("Ang2")), have been identified. Knock-out and transgenic manipulation of the expression of Tie-2 and its ligands indicates tight spatial and temporal control of Tie-2 signaling is essential for the proper development of new vasculature. The current model suggests that stimulation of Tie-2 kinase by the Ang1 ligand is directly involved in the branching,
20 sprouting and outgrowth of new vessels, and recruitment and interaction of periendothelial support cells important in maintaining vessel integrity and inducing quiescence. The absence of Ang1 stimulation of Tie-2 or the inhibition of Tie-2 autophosphorylation by Ang2, which is produced at high levels at sites of vascular regression, may cause a loss in vascular structure and matrix contacts resulting in
25 endothelial cell death, especially in the absence of growth/survival stimuli. The situation is however more complex, since at least two additional Tie-2 ligands (Ang3 and Ang4) have recently been reported, and the capacity for heterooligomerization of the various agonistic and antagonistic angiopoietins, thereby modifying their activity, has been demonstrated. Targeting Tie-2 ligand-receptor interactions as an
30 antiangiogenic therapeutic approach is thus less favored and a kinase inhibitory strategy preferred.

The soluble extracellular domain of Tie-2 ("ExTek") can act to disrupt the establishment of tumor vasculature in a breast tumor xenograft and lung metastasis models and in tumor-cell mediated ocular neovascularization. By adenoviral infection, the *in vivo* production of mg/ml levels ExTek in rodents may be achieved for 7-10 days with no adverse side effects. These results suggest that disruption of Tie-2 signaling pathways in normal healthy animals may be well tolerated. These Tie-2 inhibitory responses to ExTek may be a consequence of sequestration of ligand(s) and/or generation of a nonproductive heterodimer with full-length Tie-2.

Recently, significant upregulation of Tie-2 expression has been found within the vascular synovial pannus of arthritic joints of humans, consistent with a role in the inappropriate neovascularization. This finding suggests that Tie-2 plays a role in the progression of rheumatoid arthritis. Point mutations producing constitutively activated forms of Tie-2 have been identified in association with human venous malformation disorders. Tie-2 inhibitors are, therefore, useful in treating such disorders, and in other situations of inappropriate neovascularization.

The Examples herein describe the preparation and crystallization of polypeptides comprising the catalytic domain of human Tie-2. As used herein, the term "catalytic domain" refers to a specific module common to all kinases which bind ATP, such as the tyrosyl binding site, the site where ATP binds including the metal-ion binding region, and the site where the phosphoryl transfer occurs. For Tie-2, the catalytic domain is defined by amino acid residues from about residue 828 to about residue 985 of SEQ ID NO: 1, with residues 828-840, 853-855, 872, 873, 876, 879, 880, 885-888, 900, 902-909, 912, 954, 955, 960, 964, 968-971, and 980-985 included in the catalytic domain.

The amino acid sequences of native human Tie-2 (SEQ ID NO: 1) is taken as defined in SWISS-PROT (Ziegler, et al. *Oncogene*, 8:663 (1993)). As described in the Examples, certain of these crystals were examined by x-ray crystallography and atomic coordinates for the peptide were obtained. In certain cases, the polypeptide was unligated, that is, not complexed with a ligand. In other cases, the polypeptide was complexed with a ligand and the atomic coordinates of the ligand bound to the Tie-2 catalytic domain were also obtained.

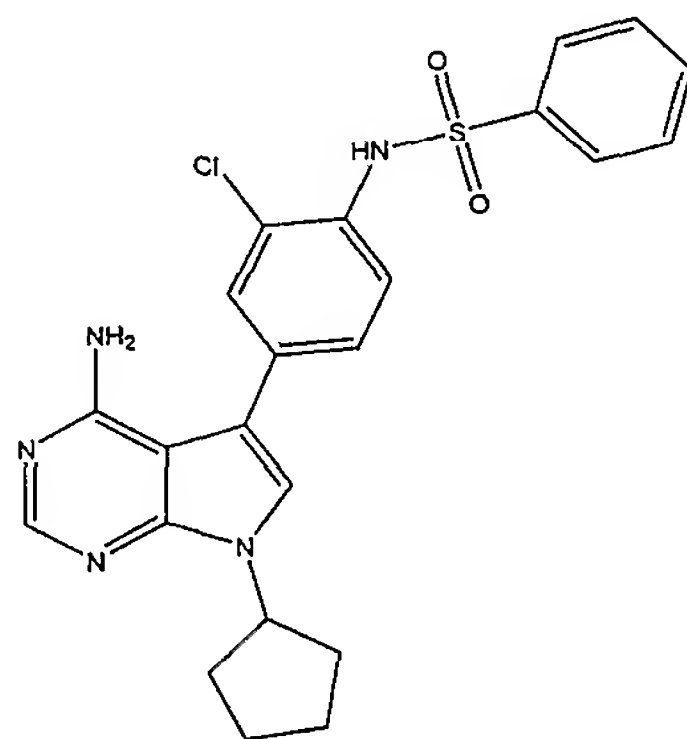
Tie-2 is subject to autophosphorylation and transphosphorylation by other proteins. Phosphorylation state is a particularly important posttranslational modification to consider. A wild-type construct (i.e., without the D964N mutation) having residues 802-1124 of SEQ ID NO 1 was isolated from an expression system as
5 a singly- or a multiply-phosphorylated species. One singly-phosphorylated species has its phosphate on either Y897 or Y899. In multiply phosphorylated species, phosphorylation can be on combinations of many Y residues on the protein. A diphosphorylated species crystallized in the space group P2(1)2(1)2(1) with the unit cell dimensions of $a = 54.320 \text{ \AA}$, $b = 75.872 \text{ \AA}$, $c = 78.143 \text{ \AA}$, and $\alpha = \beta = \gamma = 90.0^\circ$.
10 The term "space group" is a term of art which refers to the collection of symmetry elements of the unit cell of a crystal. Other phosphorylation sites are described in Jones, N., *et al.*, *J. Biol. Chem.* (1999), 274(43):30896.

A catalytically inactive mutant of human Tie-2 (SEQ ID NO 2) was also crystallized. The catalytically inactive mutant had the same sequence as residues 802
15 to 1124 of human Tie-2 except that residue 964 which is aspartic acid in wild type human Tie-2 was replaced with asparagine. This substitution rendered the mutant catalytically inactive. SEQ ID NO 2 crystallized in the space group C222(1) which had the unit cell dimensions $a = 75.195 \text{ \AA}$, $b = 116.287 \text{ \AA}$, $c = 95.060 \text{ \AA}$, and $\alpha = \beta = \gamma = 90.0^\circ$.

20 The atomic coordinates for four crystals of Tie-2/ligand complexes examined by x-ray crystallography are presented in Figs. 3A-3OO, 4A-4OO, 5A-5RR and 6A-6NN. The term "atomic coordinates" (or "structural coordinates") refers to mathematical coordinates derived from mathematical equations related to the patterns obtained on diffraction of x-rays by atoms (scattering centers) of a crystalline
25 polypeptide comprising a Tie-2 catalytic domain molecule. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal. Atomic coordinates can be transformed as is known in the art to different coordinate systems without affecting the relative positions of the
30 atoms.

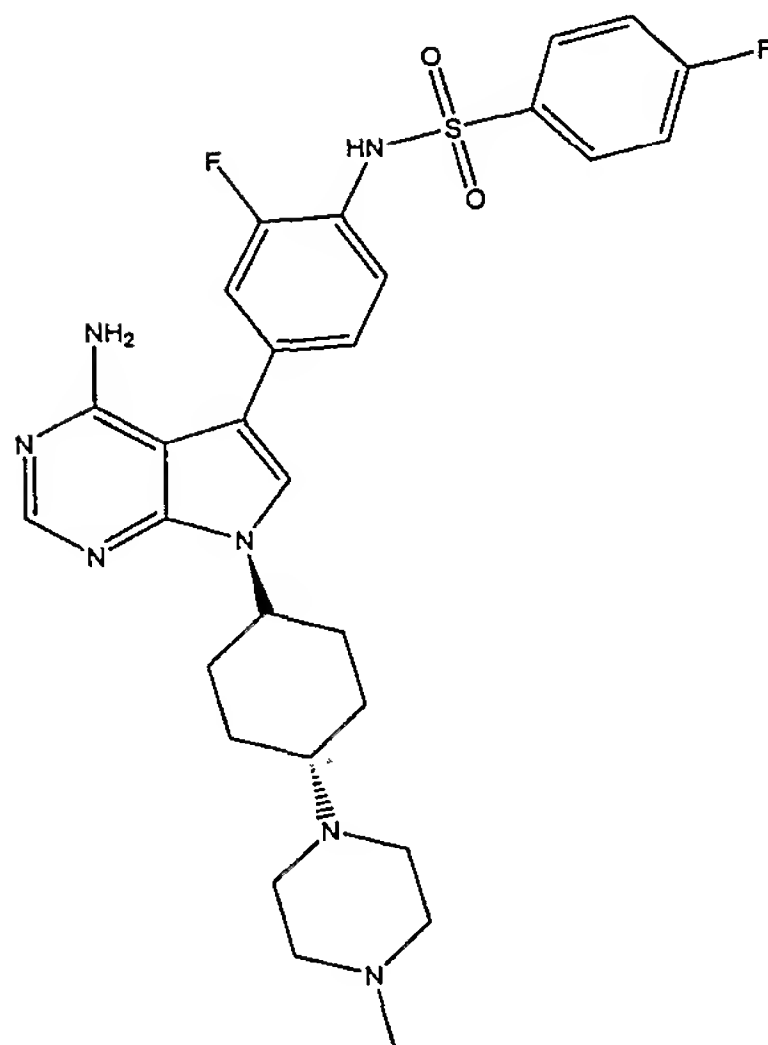
In particular, four high resolution crystal structures were obtained for SEQ ID NO 2) complexed with one of four different inhibitors shown below:

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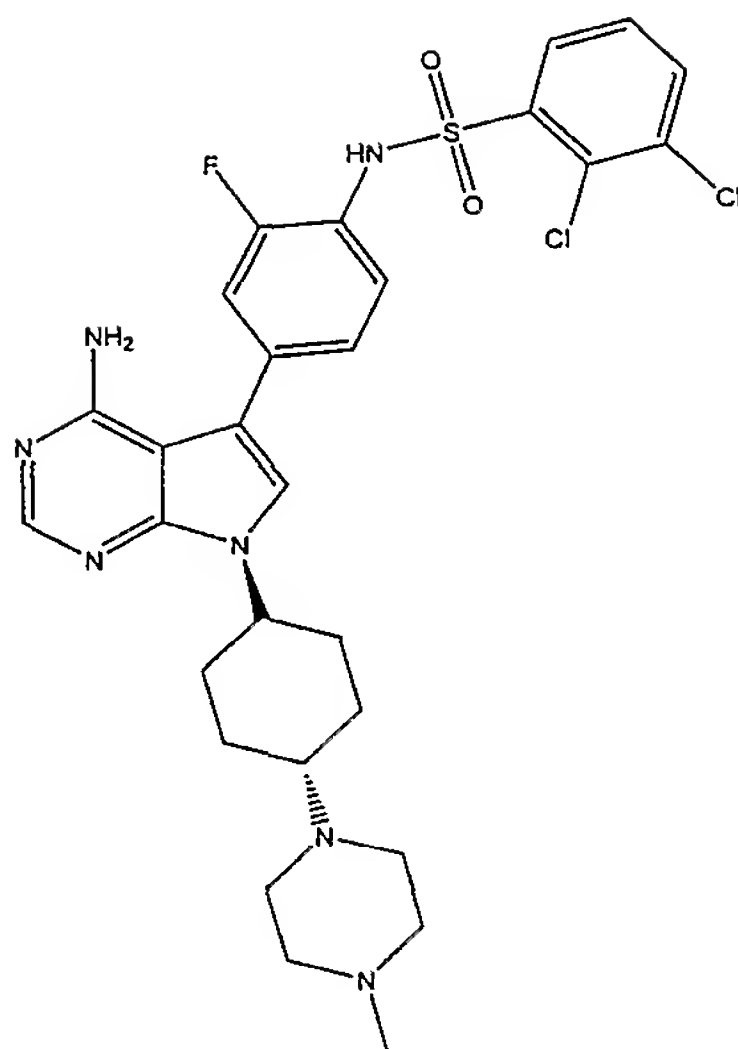
Inhibitor I

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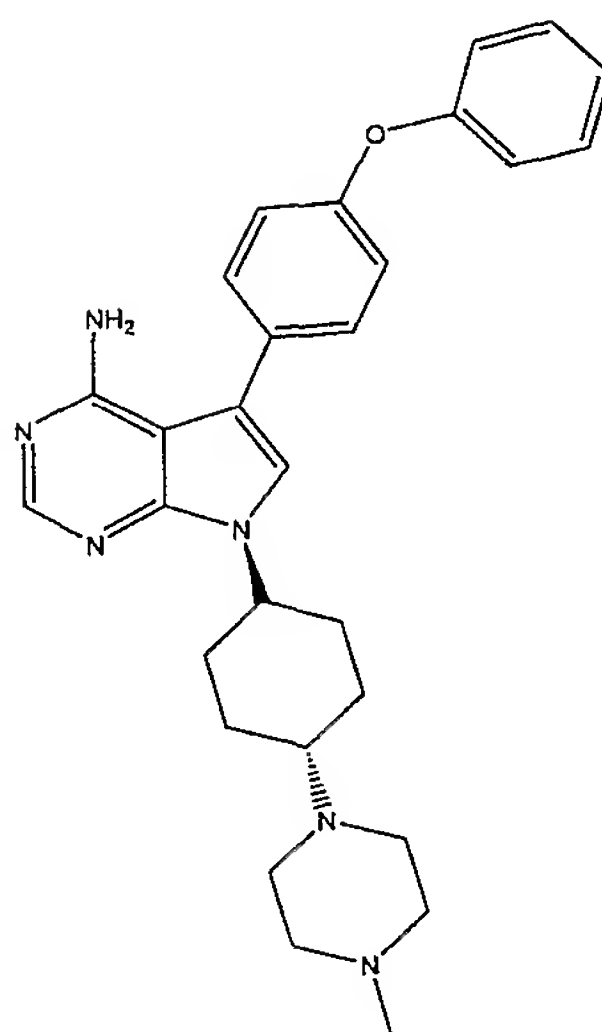
Inhibitor II

-12-



Inhibitor III

5



Inhibitor IV

The results of the x-ray crystal structure determination for SEQ ID NO 2, the
10 catalytic domain of human Tie-2, showed the following features:

The overall structure adopted a recognizable kinase fold with an N-terminal lobe and a somewhat larger C-terminal lobe. ATP binding was at the interface of the two lobes with inhibitors also binding in this region. The major secondary structural elements of the N-terminal lobe were a five strand beta sheet and a long alpha helix. The C-terminal lobe was primarily a bundle of alpha helices with a short, two-strand beta sheet near the interface with the N-terminal lobe. Fig. 7 shows a prototypical receptor tyrosine kinase, insulin receptor kinase which highlights the structural features associated with known kinases. The structure of the catalytic domain of Tie-2, shown in Fig. 9 has similar features to this

The hinge region connects the N-terminal and C-terminal lobes. The portion of the hinge which forms part of the ATP/inhibitor binding region presents several hydrogen bonding partners. The carbonyl oxygen atoms of E903, A905 and P906 and the backbone amide protons of A905, H907 and G908 were presented into the pocket. The sidechains of L900, I902, Y904 and A905 helped to define the size, shape and nature of the binding pocket.

The purine core binding region was the region where the N-terminal and C-terminal lobes of the protein cooperate to form a flat, predominantly hydrophobic binding region which is the traditional location for the purine ring of ATP in other kinase structures. The residues which contribute to this region included: I830, A853, V838, I886, L971 and A981. Sidechains of residues in the hinge region, I902, Y904 and A905 also contributed hydrophobic character to this region. The carbonyl oxygen of I830 and the amide proton of V838 also presented an interaction site within this region.

By analogy to known kinase structures, the ribose ring of ATP would traditionally occupy an area between G831 in the N-terminal lobe and N909 in the C-terminal lobe called the extended sugar pocket. The backbone amide protons of G831, E832 and N909, the carbonyl oxygen of R968 and the sidechains of E832, N909 and D912 presented hydrogen bond partners.

By analogy to known kinase structures, the γ -phosphate of ATP would occupy an area around the sidechains of residues D964 (N964 in the catalytically inactive mutant, SEQ ID NO 2). The sidechain of R968 also contributes to this

region. The predominant available interaction type was hydrogen bonding, with quite complex coordination possible.

The nucleotide binding loop, or glycine-rich loop, was a flap like loop in the N-terminal lobe which covered the front portion of the ATP binding region. Residues not already described in other binding areas include D828, V829, G833, N834, F835, G836, Q837, L839, and K840. Residues I830, G831, E832 and V838 were also part of this structural element, but have already been included in other binding regions described above. This loop is usually considered to be very flexible and is capable of altering the shape and size of the ATP binding region. Carbonyl oxygen atoms, N834 sidechain atoms and backbone amide protons of G833, N834 and F835 were potentially available for hydrogen bonding. The sidechain atoms of D828 and K840 were available for ionic/hydrogen bonding interactions. The sidechain atoms of V829, I830, F835 and L839 can contribute to hydrophobic interactions.

The early activation loop was a long flexible loop containing at least one residue, the phosphorylation of which, is generally believed to determine the activation state of the protein. The loop begins in the ATP binding site and ends in the C-terminal lobe in the area which most likely corresponds to substrate binding. Residues F983, G984, and L985 form part of the ATP binding site and were also on the N-terminal side of the activation loop. The carboxyl oxygen and amide protons of F983 and G984 and the amide proton of L985 were available for hydrogen bonding and the sidechains of F983 and L985 can contribute to hydrophobic interactions.

K855, by homology to known kinases, is part of the catalytic mechanism of the kinase. The amino group can participate in ionic or hydrogen bond interactions and the methylene groups can contribute to hydrophobic interactions. The sidechain is very mobile.

The distal hydrophobic pocket is characterized by a buried hydrophobic cavity. This portion of the ATP binding region is not occupied by any ATP atoms in known kinase structures. Residues which contribute to this pocket include L873, L876, L879, I885, L888, Y954, L955, F960 and I980. I886, A981 and F983 from regions already described also contribute hydrophobic interactions to this region. In addition, there was a number of backbone hydrogen bond partners available in this

area. These partners included the carbonyl oxygen atoms of I886, L879, and G880. With the apparent disruption of the alpha-C helix, carbonyl oxygen atoms of E872, L873 and L876 may also be available. The backbone amide proton of residues, I886 and L888 were also available in this region.

5 Several residues contributed to the ATP/inhibitor binding site but do not seem to be part of definable subregion. These residues are I854, E872, N887, I970 and I980. E872 often forms an ionic interaction with the catalytic lysine in known kinase structures. N887 may contribute to the distal hydrophobic pocket. The sidechains of I854, and I970 face away from the ATP pocket, however carbonyl oxygen atoms from
10 these residues as well as I980 were presented towards the binding region.

 The structure of the SEQ ID NO 2/inhibitor I complex had the following features:

 Final resolution of the structure was 2.8 Å in space group C2221, with final coordinates determined for backbone atoms of residues 818-857, 864-995, 1001-1116.

15 The pyrrolopyrimidine ring of inhibitor I formed hydrogen bonds to residues in the hinge region and interacts with purine core region. The core of the inhibitor presented a hydrogen bond donor in the form of the amino proton of the 4-NH₂ substituent to the carbonyl oxygen of E903. Atom N3 of the pyrimidine ring accepted a hydrogen bond from the backbone N-H of A905. The ring system of the core
20 presented a planar face to residues of both the C-terminal and N-terminal lobes. The residues in these areas present a hydrophobic surface which "sandwiches" the planar core of the inhibitor. Residues involved in this hydrophobic sandwich region include I830, V838, I86, I902 and L971. Atoms N1 and N7 of the inhibitor core faced the solvent exposed mouth of the binding pocket. Atom C6 of the inhibitor faced the long
25 axis of the nucleotide binding loop of the N-terminal lobe of the protein.

 The N7 cyclopentane ring of Inhibitor I was directed towards solvent but was still within the protein cavity. This region was described above as the extended sugar pocket. This region was characterized by hydrophobic interactions with primarily I830 and L971. Methylene groups of E832 may also contribute in this fashion.

30 The phenyl ring attached to C5 of the pyrrolopyrimidine ring was in a predominantly hydrophobic area, generated by residues from the purine core region,

the distal hydrophobic pocket and methylene groups from the catalytic lysine, K855. The hydrophobic contacts were with residues V838, I886, I902, L971 and A981. Lysine 855 was highly mobile, so it is also possible that the chlorine atom meta to the pyrrolopyrimidine ring was receiving a hydrogen bond.

5 The sulfonamide linker made a clear hydrogen bond with an amide proton of D982 and may also make a hydrogen bond to the amide proton of F983.

 The terminal phenyl ring was located in the distal hydrophobic pocket. Primary contacts were with L876, I886, L888 and F983.

 The structure of the SEQ ID NO 2/inhibitor II, SEQ ID NO 2/inhibitor III and
10 SEQ ID NO 2/inhibitor IV complexes had the following features:

 Residues 818-857, 864-995, 1001-1116 have been modeled into the solved structure. A space group P42212 was observed. The overall fold is still a standard kinase catalytic domain fold and the binding regions described above for SEQ ID NO 2/inhibitor I still pertain.

15 The pyrrolopyrimidine core, B-ring, linker and C-ring of inhibitor II in the SEQ ID NO 2/inhibitor II complex was bound the same way as inhibitor I. In addition, the N-7 cyclohexyl N-methyl piperazinyl group occupied the extended sugar pocket and made a strong ionic interaction with D912.

 The pyrrolopyrimidine of inhibitor III binds was bound the same way in the
20 SEQ ID NO 2/inhibitor III complex as inhibitor I. The N-7 cyclohexyl N-methyl piperazinyl group occupied the extended sugar pocket and made a strong ionic interaction with D912 as in the SEQ ID NO 2/inhibitor II complex. The B-ring was bound in a similar fashion to inhibitor I, however, the hydrogen bond between halogens, fluorine in this case, and K855 was more clear. The sulfonyl oxygens of the
25 sulfonamide linker made two clear hydrogen bonds to backbone amide protons of D983 and F983. The C-ring occupied the distal hydrophobic pocket with main interactions coming from L876, I886, L888, L900, I902 and F983.

 The pyrrolopyrimidine core of inhibitor IV in the SEQ ID NO 2/inhibitor IV complex was bound the same way as inhibitor I. The N-7 cyclohexyl N-methyl
30 piperazinyl group occupies the extended sugar pocket and makes a strong ionic interaction with D912 as in SEQ ID NO 2/inhibitor II. The B-ring binds in a similar

fashion to inhibitor I, however there is no halogen atom to act as a potential hydrogen bond partner in inhibitor IV. The oxygen atom of the linker accepted a hydrogen bond from the catalytic lysine, K855. The C-ring of inhibitor IV occupied the distal hydrophobic pocket with main interactions coming from L876, I886, I902 and F983.

- 5 Analysis of the three dimensional structure of the Tie-2 catalytic domain has indicated the presence of a number of subsites, each of which includes molecular functional groups capable of interacting with complementary moieties of an inhibitor. Subsites 1 through 9 of the Tie-2 catalytic domain are defined below. A summary of the properties of the chemical moieties present at each subsite is given below.
- 10 Subsites are characterized below according to the properties of chemical moieties with which they are complementary, or with which they can interact. Such moieties can include hydrogen bond acceptors, such as hydroxyl, amino, ether, thioether, carboxyl, P=O, and carbonyl groups, halogen atoms, such as fluorine, chlorine, bromine and iodine atoms; and other groups including a heteroatom having at least one lone pair of
- 15 electrons, such as groups containing trivalent phosphorous, di- and tetravalent sulfur, oxygen and nitrogen atoms; hydrogen bond donors, such as hydroxyl, thiol, an amide proton, amine protons, carboxylic acid groups and any of the groups listed under hydrogen atom acceptors to which a hydrogen atom is bonded; hydrophobic groups, such as linear, branched or cyclic alkyl, ether or thioalkyl groups; linear, branched or
- 20 cyclic alkenyl groups; linear, branched or cyclic alkynyl groups; aryl groups, such as mono- and polycyclic aromatic hydrocarbyl groups and mono- and polycyclic heterocyclic or heteroaryl groups; positively charged groups, such as primary, secondary, tertiary and quaternary ammonium groups, imidazolium and other protonated heteroalkyl and heteroaryl moieties, substituted and unsubstituted
- 25 guanidinium groups, sulfonium groups and phosphonium groups; and negatively charged groups, such as carboxylate, phenolate, thiolate, sulfonamide, sulfamate, boronate, vanadate, sulfonate, sulfinde, phosphinate, tetrazolate and other heteroaryl anions, heterocyclic N-oxides, and phosphonate groups. A given chemical moiety can contain one or more of these groups.

Subsite 1: Hinge Region

Hydrogen Acceptors: The the backbone carbonyl oxygen of residues E903, A905 and P906 present proton acceptors.

5 Hydrogen Donors: The backbone amide protons of residues A905, H907 and G908 present proton donors.

Hydrophobic Groups: The sidechains of L900, I902, Y904 and A905 present hydrophobic groups.

Subsite 2: The Purine Core Binding Region

10 Hydrophobic Groups: Residues I830, A853, V838, I886, L971, A981 and the sidechains of residues I902, Y904, and A905 present hydrophobic groups.

Hydrogen Acceptors: The carbonyl oxygen of I830 presents a proton acceptor.

Hydrogen Donors: The amide proton of V838 presents a proton donor.

15 Subsite 3: The Extended Sugar Pocket

Hydrogen Acceptors: The backbone carbonyl oxygen of R968 and the sidechain carbonyl oxygen of E832, N909 and D912 present proton acceptors.

Hydrogen Donors: The backbone amide protons of G831, E832 and N909 present proton donors.

20

Subsite 4: The Extended γ -Phosphate Region

Hydrogen Bonding Groups: Residues D964 (N964 in the catalytically inactive mutant), N969 and D982 present both proton donor and proton acceptor groups.

25 Subsite 5: The Nucleotide binding Loop

Hydrogen Acceptors: The carbonyl oxygen of the sidechain of residue N834 presents a proton acceptor.

Hydrogen Donors: The backbone amide protons of residues G833, N834 and F835 present proton donors.

30 Positively Charged Group: The sidechain of K840 presents a positively charged site.

Negatively Charged Group: The sidechain of D828 presents a negatively charged site.

Hydrophobic Groups: The sidechains of V829, I830, F835 and L839 present hydrophobic groups.

Subsite 6: The Early Activation Loop

5 Hydrogen Acceptors: The backbone carbonyl oxygens of residues F983 and G984 presents a proton acceptor.

Hydrogen Donors: The backbone amide protons of residues F983, G984 and L985 present proton donors.

10 Hydrophobic Groups: The sidechains of F983 and L985 present hydrophobic groups.

Subsite 7: The Catalytic Lysine

Positively Charged Group: The sidechain of K855 presents a positively charged site.

Hydrophobic Group: The methylene groups of the sidechain of K855 presents a hydrophobic group.

15

Subsite 8: The Distal Hydrophobic Pocket

Hydrophobic Groups: Residues L873, L876, L879, I885, L888, Y954, L955, F960, I980, I886, A981 and F983 present hydrophobic groups.

20 Hydrogen Acceptors: The backbone carbonyl oxygens of residues I886, L879, G880, E872, L873 and L876 present proton acceptors.

Hydrogen Donors: The backbone amide protons of residues I886 and L888 present proton donors.

Subsite 9: Miscellaneous interaction sites which contribute to the ATP binding site.

25 Hydrogen Acceptors: The backbone carbonyl oxygens of residues I854, I970 and I980 present proton acceptors in the ATP binding region.

Negatively Charged Groups: E872 presents a negatively charged group which often forms an ionic bond with the catalytic lysine residue K855.

30 Fig. 9 provides a model of the catalytic domain of Tie-2 bound to inhibitor I. Subsites 1-9 of the catalytic domain are each depicted in a different color as follows:

the hinge region (dark blue), the purine core (light blue), the extended sugar pocket (light purple), the γ -phosphate region (dark yellow), the nucleotide binding loop (red), the early activation loop (dark green), the catalytic lysine (light green), the distal hydrophobic pocket (dark purple), and miscellaneous interaction sites (brown). The inhibitor is depicted in light yellow.

In one embodiment, the present invention provides polypeptides comprising the catalytic domain of Tie-2, crystalline forms of these polypeptides, optionally complexed with a ligand, and the three dimensional structure of the polypeptides, including the three dimensional structure of the Tie-2 catalytic domain. In general, these three dimensional structures are defined by atomic coordinates derived from x-ray crystallographic studies of the polypeptides. The catalytic domain can be unphosphorylated, monophosphorylated or multiply phosphorylated. Phosphorylation typically occurs at tyrosine residues. One monophosphorylated species has a phosphate group on Y897 or Y899.

The polypeptides can include the catalytic domain of Tie-2 from any species, such as a yeast or other unicellular organism, an invertebrate or a vertebrate. Preferably, the polypeptide includes the catalytic domain of a mammalian Tie-2, such as murine Tie-2. More preferably, the polypeptide includes the catalytic domain of human Tie-2. The polypeptides of the invention also includes polypeptides comprising single nucleotide polymorphisms of the catalytic domain of human Tie-2 or murine Tie-2. In one embodiment, the polypeptides of the invention, and crystalline forms thereof, include a sequence which has at least 80% identity to the catalytic domain of human Tie-2 or murine Tie-2.

To determine the percent identity of two amino acid sequences, the sequences are aligned for optimal comparison purposes (*e.g.*, gaps can be introduced in one or both of a first and a second amino acid or nucleic acid sequence for optimal alignment, and non-homologous (dissimilar) sequences can be disregarded for comparison purposes). In a preferred embodiment, the length of a first sequence aligned for comparison purposes is at least 30%, preferably at least 40%, more preferably at least 50%, even more preferably at least 60%, and even more preferably at least 70%, 80%, or 90% of the length of the second sequence. The amino acid

residues at corresponding amino acid positions are then compared. When a position in the first sequence is occupied by the same amino acid residue as the corresponding position in the second sequence, then the molecules are identical at that position. The percent identity between the two sequences is a function of the number of identical positions shared by the sequences, taking into account the number of gaps, and the length of each gap, which need to be introduced for optimal alignment of the two sequences.

The invention also encompasses polypeptides having a lower degree of identity but having sufficient homology so as to perform one or more of the same functions performed by Tie-2 polypeptides described herein by amino acid sequence. Homology for a polypeptide is determined by conservative amino acid substitution. Such substitutions are those that substitute a given amino acid in a polypeptide by another amino acid of like characteristics. Conservative substitutions are likely to be phenotypically silent. Typically seen as conservative substitutions are the replacements, one for another, for example, among the aliphatic amino acids Ala, Val, Leu, and Ile; interchange of the hydroxyl residues Ser and Thr, exchange of the acidic residues Asp and Glu, substitution between the amide residues Asn and Gln, exchange of the basic residues Lys and Arg or replacements among the aromatic residues Phe, Tyr and Trp. Guidance concerning which amino acid changes are likely to be phenotypically silent is found in Bowie *et al.*, *Science* 247:1306-1310 (1990).

The comparison of sequences and determination of percent identity and homology between two sequences can be accomplished using a mathematical algorithm. (*Computational Molecular Biology*, Lesk, A.M., ed., Oxford University Press, New York, 1988; *Biocomputing: Informatics and Genome Projects*, Smith, D.W., ed., Academic Press, New York, 1993; *Computer Analysis of Sequence Data, Part 1*, Griffin, A.M., and Griffin, H.G., eds., Humana Press, New Jersey, 1994; *Sequence Analysis in Molecular Biology*, von Heinje, G., Academic Press, 1987; and *Sequence Analysis Primer*, Gribskov, M. and Devereaux, J., eds., M. Stockton Press, New York, 1991). In a preferred embodiment, the percent identity between two amino acid sequences is determined using the Needleman and Wunsch (*J. Mol. Biol.* (48):444-453 (1970)) algorithm which has been incorporated into the GAP program in

the GCG software package (available on March 29, 2000 at <http://www.gcg.com>), using either a Blossum 62 matrix or a PAM250 matrix, and a gap weight of, for example, 16, 14, 12, 10, 8, 6, or 4 and a length weight of, for example, 1, 2, 3, 4, 5, or 6. In yet another preferred embodiment, the percent identity between two nucleotide sequences is determined using the GAP program in the GCG software package (Devereux, J., *et al.*, *Nucleic Acids Res.* 12(1):387 (1984)) (available on March 29, 2000 at <http://www.gcg.com>), using a NWSgapdna.CMP matrix and a gap weight of, for example, 40, 50, 60, 70, or 80 and a length weight of, for example, 1, 2, 3, 4, 5, or 6. In another embodiment, the percent identity between two amino acid or nucleotide sequences is determined using the algorithm of E. Meyers and W. Miller (*CABIOS*, 4:11-17 (1989)) which has been incorporated into the ALIGN program (version 2.0), using, for example, a PAM120 weight residue table, a gap length penalty of 12 and a gap penalty of 4.

The protein sequences of the present invention, for example, amino acids 802-1124 of human Tie-2 (SEQ ID NO 1), can further be used as a "query sequence" to perform a search against databases to, for example, identify other family members or related sequences. Such searches can be performed using the NBLAST and XBLAST programs (version 2.0) of Altschul, *et al.* (*J. Mol. Biol.* 215:403-10 (1990)). BLAST protein searches can be performed with the XBLAST program, for example, score = 50, word length = 3, to obtain amino acid sequences homologous to the proteins of the invention. To obtain gapped alignments for comparison purposes, gapped BLAST can be utilized as described in Altschul *et al.*, (*Nucleic Acids Res.* 25(17):3389-3402 (1997)). When utilizing BLAST and gapped BLAST programs, the default parameters of the respective programs (*e.g.*, XBLAST and NBLAST) can be used as given on March 29, 2000 at <http://www.ncbi.nlm.nih.gov>.

Homology for amino acid sequences can be defined in terms of the parameters set by the Advanced Blast search available from NCBI (the National Center for Biotechnology Information; see, for Advanced BLAST, www.ncbi.nlm.nih.gov/cgi-bin/BLAST/nph-newblast?Jform=1 (on March 29, 2000)). These default parameters, recommended for a query molecule of length greater than 85 amino acid residues or nucleotides have been set as follows: gap existence cost, 11, per residue gap cost, 1;

lambda ratio, 0.85. Further explanation of version 2.0 of BLAST can be found on related website pages and in Altschul, S.F. *et al.*, *Nucleic Acids Res.* 25:3389-3402 (1997).

5 In one embodiment, the polypeptide includes amino acids 802 to 1124 of SEQ ID NO: 1. Polypeptides can also have amino acids 792 to 1124, 782 to 1124, 772 to 1124, 812 to 1124, 822 to 1124, 832 to 1124, 802 to 1114, 802 to 1104, or 802 to 1094 of SEQ ID NO 1. In another embodiment, the polypeptide can be a catalytically inactive mutant of Tie-2, such as SEQ ID NO 2, wherein the asparagine amino acid at 964 is replaced with an aspartic acid amino acid (designated D964N mutant). Other
10 catalytically inactive mutants include substitution of the asparagine amino acid at 964 with alanine, serine, threonine, or glycine.

In another embodiment, the catalytic domain which is crystallized can have deletions of amino acids from the native sequence. For example, a polypeptide which is suitable for crystallization can include amino acids 802 to 918 of SEQ ID NO 1
15 fused to amino acids 934 to 1124 of SEQ ID NO 1 or other related "kinase-insert domain" deletions.

The crystalline polypeptide, preferably, further includes a ligand bound to the Tie-2 catalytic domain. The ligand is, preferably, a small (less than about 1500 molecular weight) organic molecule, for example, inhibitor I, II, III, or IV.

20 In one embodiment, the invention relates to a method of determining the three dimensional structure of a first polypeptide comprising the catalytic domain of a Tie-2 protein. The method includes the steps of (1) obtaining a crystal comprising the first polypeptide; (2) obtaining x-ray diffraction data for said crystal; and (3) using the x-ray diffraction data and the atomic coordinates of a second polypeptide comprising the
25 catalytic domain of a Tie-2 protein to solve the crystal structure of the first polypeptide, thereby determining the three dimensional structure of the first polypeptide. The second polypeptide can include the same Tie-2 catalytic domain as the first polypeptide, or a different Tie-2 catalytic domain. Either or both of the first and second polypeptides can, optionally, be complexed with a ligand. That is, the
30 crystal of the first polypeptide can comprise a complex of the first polypeptide with a ligand. The atomic coordinates of the second polypeptide can, optionally, include the

atomic coordinates of a ligand molecule bound to the second polypeptide. The atomic coordinates of the second polypeptide, generally, have been previously obtained, for example, by x-ray crystallographic analysis of a crystal comprising the second polypeptide or a complex of the second polypeptide with a ligand. The atomic
5 coordinates of the second polypeptide can be used to solve the crystal structure using methods known in the art, for example, molecular replacement or isomorphous replacement. Preferably, the second polypeptide comprises the catalytic domain of a mammalin Tie-2, more preferably, human Tie-2. For example the atomic coordinates which can be used include the atomic coordinates presented herein, preferably the
10 atomic coordinates presented in Figures 3-7.

The invention also provides a method of identifying a compound which is a potential inhibitor of Tie-2. The method comprises the steps of (1) obtaining a crystal of a polypeptide comprising the catalytic domain of Tie-2; (2) obtaining the atomic coordinates of the polypeptide by x-ray diffraction studies using said crystal; (3) using
15 said atomic coordinates to define the catalytic domain of Tie-2; and (4) identifying a compound which fits the catalytic domain. The method can further include the steps of obtaining, for example, from a compound library, or synthesizing the compound identified in step 4, and assessing the ability of the identified compound to inhibit Tie-2 enzymatic activity.

20 The polypeptide preferably comprises the catalytic domain of a mammalian Tie-2. More preferably the polypeptide comprises the catalytic domain of human Tie-2. In a preferred embodiment, the polypeptide is a polypeptide of the present invention, as described above.

The polypeptide can be crystallized using methods known in the art, such as
25 the methods described in the Examples, to afford polypeptide crystals which are suitable for x-ray diffraction studies. A crystalline polypeptide/ligand complex can be produced by soaking the resulting crystalline polypeptide in a solution including the ligand. Preferably, the ligand solution is in a solvent in which the polypeptide is insoluble.

30 The atomic coordinates of the polypeptide (and ligand) can be determined, for example, by x-ray crystallography using methods known in the art. The data obtained

from the crystallography can be used to generate atomic coordinates, for example, of the atoms of the polypeptide and ligand, if present. As is known in the art, solution and refinement of the x-ray crystal structure can result in the determination of coordinates for some or all of the non-hydrogen atoms. The atomic coordinates can be used, as is known in the art, to generate a three-dimensional structure of the Tie-2 catalytic domain. This structure can then be used to assess the ability of any given compound, preferably using computer-based methods, to fit into the catalytic domain.

A compound fits into the catalytic domain if it is of a suitable size and shape to physically reside in the catalytic domain, that is, if it has a shape which is complementary to the catalytic domain and can reside in the catalytic domain without significant unfavorable steric or van der Waals interactions. Preferably, the compound includes one or more functional groups and/or moieties which interact with one or more subsites within the catalytic domain. Computational methods for evaluating the ability of a compound to fit into the catalytic domain, as defined by the atomic coordinates of the polypeptide, are known in the art, and representative examples are provided below.

In another embodiment, the method of identifying a potential inhibitor of Tie-2 comprises the step of determining the ability of one or more functional groups and/or moieties of the compound, when present in the Tie-2 catalytic domain, to interact with one or more subsites of the Tie-2 catalytic domain. Preferably, the Tie-2 catalytic domain is defined by the atomic coordinates of a polypeptide comprising the Tie-2 catalytic domain. If the compound is able to interact with a preselected number or set of subsites, the compound is identified as a potential inhibitor of Tie-2.

A functional group or moiety of the compound is said to "interact" with a subsite of the Tie-2 catalytic domain if it participates in an energetically favorable, or stabilizing, interaction with one or more complementary moieties within the subsite. Two chemical moieties are "complementary" if they are capable, when suitably positioned, of participating in an attractive, or stabilizing, interaction, such as an electrostatic or van der Waals interaction. Typically, the attractive interaction is an ion-ion (or salt bridge), ion-dipole, dipole-dipole, hydrogen bond, pi-pi or hydrophobic interaction. For example, a negatively charged moiety and a positively

charged moiety are complementary because, if suitably positioned, they can form a salt bridge. Likewise, a hydrogen bond donor and a hydrogen bond acceptor are complementary if suitably positioned.

Typically, an assessment of interactions between the test compound and the Tie-2 catalytic domain may employ computer-based computational methods, such as those known in the art, in which possible interactions of a compound with the protein, as defined by atomic coordinates, are evaluated with respect to interaction strength by calculating the interaction energy upon binding the compound to the protein. Compounds which have calculated interaction energies within a preselected range or which otherwise, in the opinion of the computational chemist employing the method, have the greatest potential as Tie-2 inhibitors, can then be provided, for example, from a compound library or via synthesis, and assayed for the ability to inhibit Tie-2. The interaction energy for a given compound generally depends upon the ability of the compound to interact with one or more subsites within the protein catalytic domain.

In one embodiment, the atomic coordinates used in the method are the atomic coordinates set forth in Figs. 3A-3OO, 4A-4OO, 5A-5RR and 6A-6NN. It is to be understood that the coordinates set forth in Figs. 3-6 can be transformed, for example, into a different coordinate system, in ways known to those skilled in the art without substantially changing the three dimensional structure represented thereby.

In certain cases, a moiety of the compound can interact with a subsite via two or more individual interactions. A moiety of the compound and a subsite can interact if they have complementary properties and are positioned in sufficient proximity and in a suitable orientation for a stabilizing interaction to occur. The possible range of distances for the moiety of the compound and the subsite depends upon the distance dependence of the interaction, as is known in the art. For example, a hydrogen bond typically occurs when a hydrogen bond donor atom, which bears a hydrogen atom, and a hydrogen bond acceptor atom are separated by about 2.5 Å and about 3.5 Å. Hydrogen bonds are well known in the art (Pimentel *et al.*, *The Hydrogen Bond*, San Francisco: Freeman (1960)). Generally, the overall interaction, or binding, between the compound and the Tie-2 catalytic domain will depend upon the number and strength of these individual interactions.

The ability of a test compound to interact with one or more subsites of the catalytic domain of Tie-2 can be determined by computationally evaluating interactions between functional groups, or moieties, of the test compound and one or more amino acid side chains in a particular protein subsite, such as subsites 1 to 9 above. Typically, a compound which is capable of participating in stabilizing interactions with a preselected number of subsites, preferably without simultaneously participating in significant destabilizing interactions, is identified as a potential inhibitor of Tie-2. Such a compound will interact with one or more subsites, preferably with two or more subsites and, more preferably, with three or more subsites.

The invention further provides a method of designing a compound which is a potential inhibitor of Tie-2. The method includes the steps of (1) identifying one or more functional groups capable of interacting with one or more subsites of the Tie-2 catalytic domain; and (2) identifying a scaffold which presents the functional group or functional groups identified in step 1 in a suitable orientation for interacting with one or more subsites of the Tie-2 catalytic domain. The compound which results from attachment of the identified functional groups or moieties to the identified scaffold is a potential inhibitor of Tie-2. The Tie-2 catalytic domain is, generally, defined by the conserved homolohous sequence when compared to other known tyrosine kinases, for example, the atomic coordinates set forth in Figs. 3A-3OO, 4A-4OO, 5A-5RR and 6A-6NN.

Suitable methods, as are known in the art, can be used to identify chemical moieties, fragments or functional groups which are capable of interacting favorably with a particular subsite or set of subsites. These methods include, but are not limited to: interactive molecular graphics; molecular mechanics; conformational analysis; energy evaluation; docking; database searching; pharmacophore modeling; de novo design and property estimation. These methods can also be employed to assemble chemical moieties, fragments or functional groups into a single inhibitor molecule. These same methods can also be used to determine whether a given chemical moiety, fragment or functional group is able to interact favorably with a particular subsite or set of subsites.

In one embodiment, the design of potential human Tie-2 inhibitors begins from the general perspective of three-dimensional shape and electrostatic complementarity for the catalytic domain, encompassing subsites 1-9, and subsequently, interactive molecular modeling techniques can be applied by one skilled in the art to visually inspect the quality of the fit of a candidate inhibitor modeled into the binding site. Suitable visualization programs include INSIGHTII (Molecular Simulations Inc., San Diego, CA), QUANTA (Molecular Simulations Inc., San Diego, CA), SYBYL (Tripos Inc., St Louis, MO), RASMOL (Roger Sayle *et al.*, *Trends Biochem. Sci.* **20**: 374-376 (1995)), GRASP (Nicholls *et al.*, *Proteins* **11**: 281-289 (1991)), and MIDAS (Ferrin *et al.*, *J. Mol. Graphics* **6**:13-27 (1988)).

A further embodiment of the present invention utilizes a database searching program which is capable of scanning a database of small molecules of known three-dimensional structure for candidates which fit into the target protein site. Suitable software programs include CATALYST (Molecular Simulations Inc., San Diego, CA), UNITY (Tripos Inc., St Louis, MO), FLEXX (Rarey *et al.*, *J. Mol. Biol.* **261**: 470-489 (1996)), CHEM-3DBS (Oxford Molecular Group, Oxford, UK), DOCK (Kuntz *et al.*, *J. Mol. Biol* **161**: 269-288 (1982)), and MACCS-3D (MDL Information Systems Inc., San Leandro, CA). It is not expected that the molecules found in the search will necessarily be leads themselves, since a complete evaluation of all interactions will necessarily be made during the initial search. Rather, it is anticipated that such candidates might act as the framework for further design, providing molecular skeletons to which appropriate atomic replacements can be made. Of course, the chemical complementarity of these molecules can be evaluated, but it is expected that the scaffold, functional groups, linkers and/or monomers may be changed to maximize the electrostatic, hydrogen bonding, and hydrophobic interactions with the enzyme. Goodford (Goodford *J Med Chem* **28**:849-857 (1985)) has produced a computer program, GRID, which seeks to determine regions of high affinity for different chemical groups (termed probes) on the molecular surface of the binding site. GRID hence provides a tool for suggesting modifications to known ligands that might enhance binding.

A range of factors, including electrostatic interactions, hydrogen bonding, hydrophobic interactions, desolvation effects, conformational strain or mobility, chelation and cooperative interaction and motions of ligand and enzyme, all influence the binding effect and should be taken into account in attempts to design bioactive inhibitors.

Yet another embodiment of a computer-assisted molecular design method for identifying inhibitors comprises searching for fragments which fit into a binding region subsite and link to a predefined scaffold. The scaffold itself may be identified in such a manner. Programs suitable for the searching of such functional groups and monomers include LUDI (Boehm, *J Comp. Aid. Mol. Des.* 6:61-78 (1992)), CAVEAT (Bartlett *et al.* in "Molecular Recognition in Chemical and Biological Problems", special publication of *The Royal Chem. Soc.*, 78:182-196 (1989)) and MCSS (Miranker *et al. Proteins* 11: 29-34 (1991)).

Yet another embodiment of a computer-assisted molecular design method for identifying inhibitors of the subject phosphatase comprises the *de novo* synthesis of potential inhibitors by algorithmic connection of small molecular fragments that will exhibit the desired structural and electrostatic complementarity with the active site of the enzyme. The methodology employs a large template set of small molecules which are iteratively pieced together in a model of the Tie-2 active site. Programs suitable for this task include GROW (Moon *et al. Proteins* 11:314-328 (1991)) and SPROUT (Gillet *et al. J Comp. Aid. Mol. Des.* 7:127 (1993)).

In yet another embodiment, the suitability of inhibitor candidates can be determined using an empirical scoring function, which can rank the binding affinities for a set of inhibitors. For an example of such a method see Muegge *et al.* and references therein (Muegge *et al., J Med. Chem.* 42:791-804 (1999)).

Other modeling techniques can be used in accordance with this invention, for example, those described by Cohen *et al. (J. Med. Chem.* 33: 883-894 (1994)); Navia *et al. (Current Opinions in Structural Biology* 2: 202-210 (1992)); Baldwin *et al. (J. Med. Chem.* 32: 2510-2513 (1989)); Appelt *et al. (J. Med. Chem.* 34: 1925-1934 (1991)); and Ealick *et al. (Proc. Nat. Acad. Sci. USA* 88: 11540-11544 (1991)).

A compound which is identified by one of the foregoing methods as a potential inhibitor of Tie-2 can then be obtained, for example, by synthesis or from a compound library, and assessed for the ability to inhibit Tie-2 *in vitro*. Such an *in vitro* assay can be performed as is known in the art, for example, by contacting Tie-2 in solution with
5 the test compound in the presence of a substrate for Tie-2. The rate of substrate transformation can be determined in the presence of the test compound and compared with the rate in the absence of the test compound. Suitable assays for Tie-2 biological activity are described in Example 4.

An inhibitor identified or designed by a method of the present invention can be
10 a competitive inhibitor, an uncompetitive inhibitor or a noncompetitive inhibitor. A "competitive" inhibitor is one that inhibits Tie-2 activity by binding fully or partially within the same region of Tie-2, as ATP, thereby directly competing with ATP for the active site of Tie-2. An "uncompetitive" inhibitor inhibits Tie-2 by binding to a different region of the enzyme than ATP. Such inhibitors bind to Tie-2 already bound
15 with ATP and not to the free enzyme. A "non-competitive" inhibitor is one that can bind to either the free or ATP bound form of Tie-2. In some instances, an inhibitor may inhibit the enzymes catalytic activity by impeding the binding of multiple substrates (e.g., ATP and tyrosyl substrates). this may be accomplished by fully or partially occluding multiple substrate binding sites, or by occupying a site which
20 allosterically or conformationally reduces affinities for substrates or blocks product release.

In another embodiment, the present invention provides Tie-2 inhibitors, and methods of use thereof, which are capable of binding to the catalytic domain of Tie-2, for example, compounds which are identified as inhibitors of at least one biological
25 activity of Tie-2 or which are designed by the methods described above to inhibit at least one biological activity of Tie-2. For example, the invention includes compounds which interact with one or more, preferably two or more, and more preferably, three or more of Tie-2 subsites 1 to 9.

In one embodiment, the Tie-2 inhibitor of the invention comprises a moiety or
30 moieties positioned to interact with subsite 1, subsite 2 and, optionally, with at least one other subsite, when present in the Tie-2 catalytic domain. For example, a

functional group which can interact with subsite 1 can be a hydrogen bond donor, a hydrogen bond acceptor, or a hydrophobic moiety. A functional group which can interact with subsite 2 can be a hydrophobic group, hydrogen bond donor, or a hydrogen bond acceptor.

5 In another embodiment, the Tie-2 inhibitor of the invention comprises functional groups positioned to interact with subsites 1, 2 and 3, and, optionally, one or more additional subsites.

 The Tie-2 inhibitors of the invention also include compounds having functional groups positioned to interact with subsite 1, subsite 2, subsite 8 and, 10 optionally, one or more additional subsites. In another embodiment, the inhibitor has functional groups positioned to interact with subsite 1, subsite 2, subsite 3, subsite 8, and, optionally, one or more additional subsites.

 In other embodiments, the Tie-2 inhibitors of the invention include compounds which have functional groups positioned to interact with the following groups of 15 subsites, each of which can, optionally, include one or more additional subsites: subsites 1, 4, and 5; subsites 1, 2, 7 and 8; subsites 1, 2, 3, 7 and 8; subsites 1, 2, 3, 7 and 8; subsites 1, 2, 4, 6 and 8; subsites 1, 2, 3, 4, 6 and 8; subsites 1, 2, 3, 4, 6 and 8.

 A moiety of the inhibitor compound is "positioned to interact" with a given subsite, if, when placed within the Tie-2 catalytic domain, as defined by the atomic 20 coordinates presented in Figs. 3-6, the moiety is proximal to, and oriented properly relative to, the appropriate amino acid side chains within the subsite.

 As indicated in the description of the subsites above, several of subsites 1-9 can potentially interact with two or more types of moieties. For each of the subsites listed below the preferred type of interacting moiety possessed by the potential 25 inhibitor is indicated.

Subsite 1: hydrogen bond donor (E903) and hydrogen bond acceptor (A905).

Subsite 2: hydrophobic, preferably aromatic, moiety (I830, V838, I886, I902 and 30 L971).

Subsite 3: hydrophobic, preferably alkyl, moiety (I830 and L971) and a positively charged moiety (D912).

Subsite 4: hydrogen acceptor moiety (D982 and F938).

5

Subsite 8: hydrophobic, preferably aromatic, moiety (L876, I886, L888 and F983)

10 A preferred Tie-2 inhibitor of the invention inhibits Tie-2 enzymatic activity with a K_i of at least about 1 mM, preferably at least about 100 μ M and more preferably at least about 10 μ M. In another embodiment, a Tie-2 inhibitor binds selectively to a Tie-2 receptor over other tyrosine kinase receptors, such as insulin receptor or Csk, KDR, lck, or zap. In a preferred embodiment, the inhibitor has a K_i 0.1 fold or less for a Tie-2 receptor than for an insulin receptor or Csk. In a more
15 preferred embodiment, the inhibitor has K_i 0.01 fold or less for a Tie-2 receptor than for an insulin receptor or Csk. In a most preferred embodiment, the inhibitor has an K_i 0.001 fold less or less for a Tie-2 receptor than for an insulin receptor or Csk.

In a preferred embodiment, the Tie-2 inhibitor of the invention comprises two or more of the following when present at, or bound to, the Tie-2 catalytic domain:
20 (a) a hydrogen bond donor positioned to interact with Glu 903 of human Tie-2; (b) a hydrogen bond acceptor positioned to interact with Ala 905 of human Tie-2; (c) a hydrogen bond donor positioned to interact with Ala 905 of human Tie-2; (d) a hydrophobic moiety positioned to interact with one or more of Ile 830, Val 838, Ala 853, Ile 886, Ile 902, Tyr 904, Ala 905 and Leu 971 of human Tie-2; (e) a hydrogen
25 bond donor or positively charged functional group positioned to interact with Asp 912 of human Tie-2; (f) a hydrogen bond donor or hydrogen bond acceptor positioned to interact with Asn 909 of human Tie-2; (g) a hydrophobic moiety positioned to interact with one or more of Val 838, Lys 855, Ile 886, Ile 902, Leu 971 and Ala 981 of human Tie-2; (h) a hydrogen bond acceptor or negatively charged functional group
30 positioned to interact with Lys 855 of human Tie-2; (i) a hydrogen bond acceptor positioned to interact with Asp 982 of human Tie-2; (j) a hydrogen bond acceptor

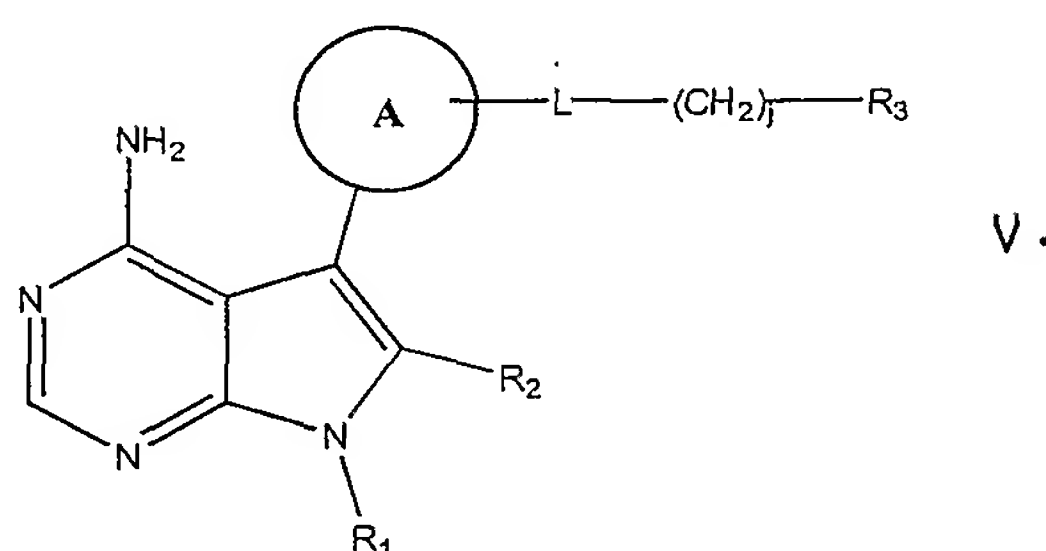
positioned to interact with Phe 983 of human Tie-2; (k) a hydrophobic moiety positioned to interact with one or more of Leu 873, Leu 876, Ile 885, Ile 886, Leu 888, Leu 900, Ile 902, Ala 981 and Phe 983 of human Tie-2; (l) a hydrogen bond donor or positively charged functional group positioned to interact with Asp 982 of human Tie-2; (m) a hydrogen bond donor positioned to interact with Ile 886 of human Tie-2; (n) a hydrogen bond donor positioned to interact with Leu 768 of human Tie-2; (o) a hydrogen bond acceptor positioned to interact with Gly 831 of human Tie-2; (p) a hydrogen bond donor or positively charged functional group positioned to interact with Glu 832 of human Tie-2; (q) a hydrogen bond acceptor or negatively charged functional group positioned to interact with Lys 840 of human Tie-2; (r) a hydrogen bond acceptor or negatively charged functional group positioned to interact with Lys 916 of human Tie-2; (s) a hydrogen bond acceptor or negatively charged functional group positioned to interact with Arg 968 of human Tie-2; (t) a hydrogen bond donor positioned to interact with Arg 968 of human Tie-2.

In preferred embodiments, the Tie-2 inhibitors of the invention comprise (b) and (d); (d) and at least one of (a), (b) and (c); (d) and at least two of (a), (b) and (c); (d) and at least two of (a), (b) and (c), and at least one of (e) and (f); (d) and (g), and at least two of (a), (b) and (c); (d), (g), at least two of (a), (b) and (c) and at least one of (e) and (f); (d), (g), (k), and at least two of (a), (b) and (c); (d), (g), (k), at least one of (e) and (f), at least two of (a), (b), and (c); (d), at least one of (i) and (j), and at least two of (a), (b) and (c); (d) and at least two of (a), (b) and (c), at least one of (e) and (f), and at least one of (i) and (j); (d), (g), (k), at least one of (i) and (j), and at least two of (a), (b) and (c); and (d), (g), (k), at least one of (e) and (f), and at least two of (a), (b) and (c).

Preferred Tie-2 inhibitors of the invention comprise a molecular scaffold or framework, to which the moieties and/or functional groups which interact with the Tie-2 subsites are attached, either directly or via an intervening moiety. The scaffold can be, for example, a peptide or peptide mimetic backbone, a cyclic or polycyclic moiety, such as a monocyclic, bicyclic or tricyclic moiety, and can include one or more hydrocarbonyl or heterocyclic rings. The molecular scaffold presents the

attached interacting moieties in the proper configuration or orientation for interaction with the appropriate residues of Tie-2.

Pyrrolopyrimidines, such as inhibitor, I, II, III or IV, are preferred Tie-2 inhibitors. Methods for synthesizing pyrrolopyrimidines are described in PCT application number WO99/21560, the teachings of which are incorporated herein by reference in their entirety. In one embodiment, the inhibitors of the invention do not include the pyrrolopyrimidines represented by structural formula V:



and pharmaceutically acceptable salts thereof, wherein:

Ring A is a six membered aromatic ring or a five or six membered heteroaromatic ring which is optionally substituted with one or more substituents selected from the group consisting of a substituted or unsubstituted aliphatic group, a halogen, a substituted or unsubstituted aromatic group, substituted or unsubstituted heteroaromatic group, substituted or unsubstituted cycloalkyl, substituted or unsubstituted heterocycloalkyl, substituted or unsubstituted aralkyl, substituted or unsubstituted heteroaralkyl, cyano, nitro, $-NR_4R_5$, $-C(O)_2H$, $-OH$, a substituted or unsubstituted alkoxycarbonyl, $-C(O)_2$ -haloalkyl, a substituted or unsubstituted alkylthio ether, a substituted or unsubstituted alkylsulfoxide, a substituted or unsubstituted alkylsulfone, a substituted or unsubstituted arylthio ether, a substituted or unsubstituted arylsulfoxide, a substituted or unsubstituted arylsulfone, a substituted or unsubstituted alkyl carbonyl, $-C(O)$ -haloalkyl, a substituted or unsubstituted aliphatic ether, a substituted or unsubstituted aromatic ether, carboxamido, tetrazolyl, trifluoromethylsulphonamido,

trifluoromethylcarbonylamino, a substituted or unsubstituted alkynyl, a substituted or unsubstituted alkyl amido, a substituted or unsubstituted aryl amido, $-NR_{95}C(O)R_{95}$, a substituted or unsubstituted styryl and a substituted or unsubstituted aralkyl amido, wherein R_{95} is an aliphatic group or an aromatic group;

5

L is $-O-$; $-S-$; $-S(O)-$; $-S(O)_2-$; $-N(R)-$; $-N(C(O)OR)-$; $-N(C(O)R)-$; $-N(SO_2R)-$; $-CH_2O-$; $-CH_2S-$; $-CH_2N(R)-$; $-CH(NR)-$; $-CH_2N(C(O)R)-$; $-CH_2N(C(O)OR)-$; $-CH_2N(SO_2R)-$; $-CH(NHR)-$; $-CH(NHC(O)R)-$; $-CH(NHSO_2R)-$; $-CH(NHC(O)OR)-$; $-CH(OC(O)R)-$; $-CH(OC(O)NHR)-$; $-CH=CH-$; $-C(=NOR)-$;

10

$-C(O)-$; $-CH(OR)-$; $-C(O)N(R)-$; $-N(R)C(O)-$; $-N(R)S(O)-$; $-N(R)S(O)_2-$; $-OC(O)N(R)-$; $-N(R)C(O)N(R)-$; $-NRC(O)O-$; $-S(O)N(R)-$; $-S(O)_2N(R)-$; $N(C(O)R)S(O)-$; $N(C(O)R)S(O)_2-$; $-N(R)S(O)N(R)-$; $-N(R)S(O)_2N(R)-$; $-C(O)N(R)C(O)-$; $-S(O)N(R)C(O)-$; $-S(O)_2N(R)C(O)-$; $-OS(O)N(R)-$; $-OS(O)_2N(R)-$; $-N(R)S(O)O-$; $-N(R)S(O)_2O-$; $-N(R)S(O)C(O)-$; $-N(R)S(O)_2C(O)-$; $-SON(C(O)R)-$; $-SO_2N(C(O)R)-$; $-N(R)SON(R)-$; $-N(R)SO_2N(R)-$; $-C(O)O-$;

15

$-N(R)P(OR')O-$; $-N(R)P(OR')-$; $-N(R)P(O)(OR')O-$; $-N(R)P(O)(OR')-$; $-N(C(O)R)P(OR')O-$; $-N(C(O)R)P(OR')-$; $-N(C(O)R)P(O)(OR')O-$ or $-N(C(O)R)P(OR')-$, wherein R and R' are each, independently, $-H$, an acyl group, a substituted or unsubstituted aliphatic group, a substituted or

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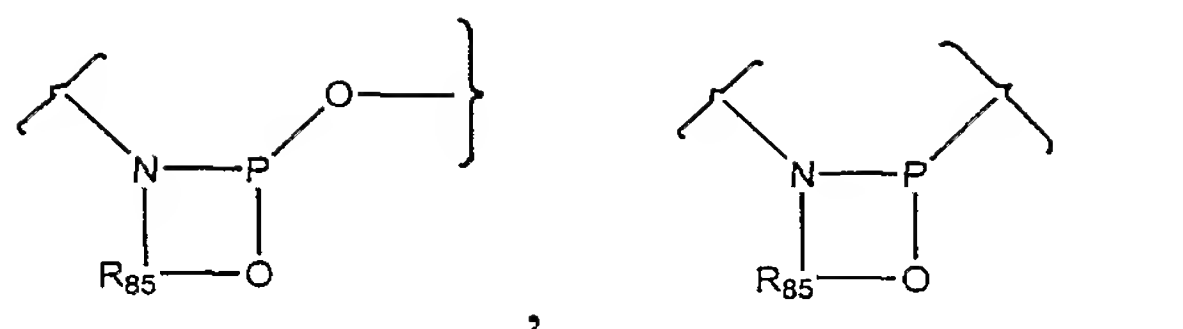
unsubstituted aromatic group, a substituted or unsubstituted heteroaromatic group, or a substituted or unsubstituted cycloalkyl group; or

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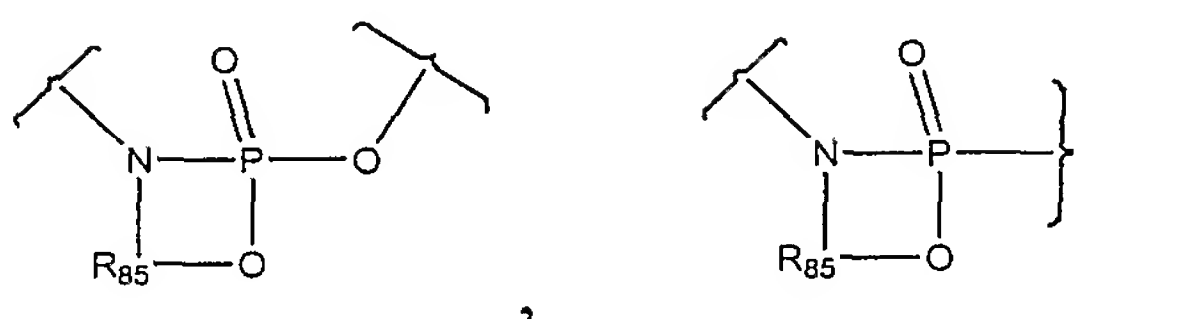
L is $-R_bN(R)S(O)_2-$, $-R_bN(R)P(O)-$, or $-R_bN(R)P(O)O-$, wherein R_b is an alkylene group which when taken together with the sulphonamide, phosphinamide, or phosphonamide group to which it is bound forms a five or six membered ring fused to ring A; or

L is represented by one of the following structural formulas:

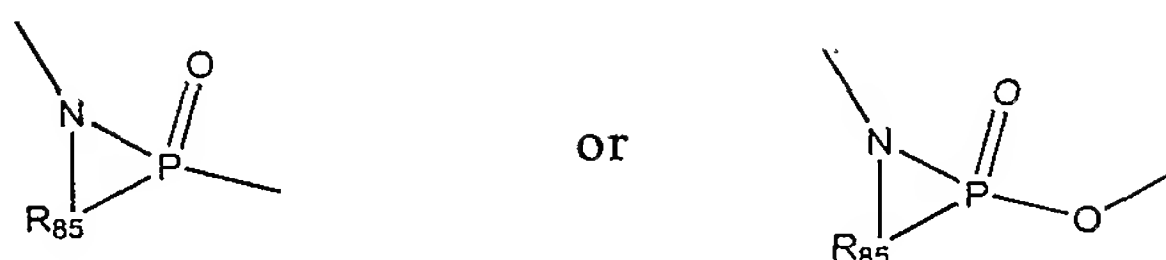
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wherein R_{85} taken together with the phosphinamide, or phosphonamide is a 5-, 6-, or 7-membered, aromatic, heteroaromatic or heterocycloalkyl ring system;

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R_1 is a substituted aliphatic group, a substituted cycloalkyl, a substituted bicycloalkyl, a substituted cycloalkenyl, an optionally substituted aromatic group, an optionally substituted heteroaromatic group, an optionally substituted heteroaralkyl, an optionally substituted heterocycloalkyl, an optionally substituted heterobicycloalkyl, an optionally substituted alkylamido, and optionally substituted arylamido, an optionally substituted $-S(O)_2$ -alkyl or optionally substituted $-S(O)_2$ -cycloalkyl, a $-C(O)$ -alkyl or an optionally substituted $-C(O)$ -alkyl, provided that when R_1 is an aliphatic group or cycloalkyl group, R_1 is not exclusively substituted with one or more substituent selected from the group consisting of hydroxyl and lower alkyl ethers, provided that the heterocycloalkyl is not 2-phenyl-1,3-dioxan-5-yl and

provided that an aliphatic group is not substituted exclusively with one or more aliphatic groups, wherein one or more substituent is selected from the group consisting of a substituted or unsubstituted aliphatic group, a substituted or unsubstituted aromatic group, a substituted or unsubstituted heteroaromatic, a substituted or unsubstituted aralkyl, a substituted or unsubstituted heteroaralkyl, a substituted or unsubstituted cycloalkyl, a substituted or unsubstituted heterocycloalkyl, a substituted or unsubstituted aromatic ether, a substituted or unsubstituted aliphatic ether, a substituted or unsubstituted alkoxycarbonyl, a substituted or unsubstituted alkylcarbonyl, a substituted or unsubstituted arylcarbonyl, a substituted or unsubstituted heteroarylcarbonyl, substituted or unsubstituted aryloxycarbonyl, -OH, a substituted or unsubstituted aminocarbonyl, an oxime, a substituted or unsubstituted azabicycloalkyl, heterocycloalkyl, oxo, aldehyde, a substituted or unsubstituted alkyl sulfonamido group, a substituted or unsubstituted aryl sulfonamido group, a substituted or unsubstituted bicycloalkyl, a substituted or unsubstituted heterobicycloalkyl, cyano, -NH₂, an alkylamino, ureido, thioureido and -B-E;

B is a substituted or unsubstituted cycloalkyl, a substituted or unsubstituted heterocycloalkyl, a substituted or unsubstituted aromatic, a substituted or unsubstituted heteroaromatic, an alkylene, an aminoalkyl, an alkylencarbonyl, or an aminoalkylcarbonyl;

E is a substituted or unsubstituted azacycloalkyl, a substituted or unsubstituted azacycloalkylcarbonyl, a substituted or unsubstituted azacycloalkylsulfonyl, a substituted or unsubstituted azacycloalkylalkyl, a substituted or unsubstituted heteroaryl, a substituted or unsubstituted heteroarylcarbonyl, a substituted or unsubstituted heteroarylsulfonyl, a substituted or unsubstituted heteroaralkyl, a substituted or unsubstituted alkyl sulfonamido, a substituted or unsubstituted aryl sulfonamido, a substituted or unsubstituted bicycloalkyl, a substituted or unsubstituted ureido, a substituted or unsubstituted thioureido or a substituted or unsubstituted aryl;

5 R_2 is $-H$, a substituted or unsubstituted aliphatic group, a substituted or unsubstituted cycloalkyl, a halogen, $-OH$, cyano, a substituted or unsubstituted aromatic group, a substituted or unsubstituted heteroaromatic group, a substituted or unsubstituted heterocycloalkyl, a substituted or unsubstituted aralkyl, a substituted or unsubstituted heteroaralkyl, $-NR_4R_5$, or $-C(O)NR_4R_5$;

R_3 is a substituted or unsubstituted aliphatic group, a substituted or unsubstituted alkenyl group, a substituted or unsubstituted cycloalkyl, a substituted or unsubstituted aromatic group, a substituted or unsubstituted heteroaromatic group, or a substituted or unsubstituted heterocycloalkyl;

10 provided that L is $-SN(R)-$, $-S(O)N(R)-$, $-S(O)_2N(R)-$, $-N(R)S-$, $-N(R)S(O)-$, $-N(R)S(O)_2-$, $-N(R)SN(R')-$, $-N(R)S(O)N(R')-$, or $-N(R)S(O)_2N(R')-$ -when R_3 is a substituted or unsubstituted aliphatic group, a substituted or unsubstituted alkenyl group;

15 provided that j is 0 when L is $-O-$, $-CH_2NR-$, $-C(O)NR-$ or $-NRC(O)-$ and R_3 is azacycloalkyl or azaheteroaryl; and

provided that j is 0 when L is $-O-$ and R_3 is phenyl;

R_4 , R_5 and the nitrogen atom together form a 3, 4, 5, 6 or 7-membered, substituted or unsubstituted heterocycloalkyl, substituted or unsubstituted heterobicycloalkyl or a substituted or unsubstituted heteroaromatic; or

20 R_4 and R_5 are each, independently, $-H$, azabicycloalkyl, heterocycloalkyl, a substituted or unsubstituted alkyl group or $Y-Z$;

Y is selected from the group consisting of $-C(O)-$, $-(CH_2)_p-$, $-S(O)_2-$, $-C(O)O-$, $-SO_2NH-$, $-CONH-$, $(CH_2)_pO-$, $-(CH_2)_pNH-$, $-(CH_2)_pS-$, $-(CH_2)_pS(O)-$, and $-(CH_2)_pS(O)_2-$;

25 p is an integer from 0 to 6;

Z is $-H$, a substituted or unsubstituted alkyl, substituted or unsubstituted amino, substituted or unsubstituted aryl, substituted or unsubstituted heteroaryl or substituted or unsubstituted heterocycloalkyl group; and

30 j an integer from 0 to 6.

As used herein, aromatic groups include carbocyclic ring systems (e.g. phenyl

and cinnamyl) and fused polycyclic aromatic ring systems (e.g. naphthyl and 1,2,3,4-tetrahydronaphthyl). Aromatic groups are also referred to as aryl groups herein.

Heteroaromatic groups, as used herein, include heteroaryl ring systems (e.g., thienyl, pyridyl, pyrazole, isoxazolyl, thiadiazolyl, oxadiazolyl, indazolyl, furans, pyrroles, imidazoles, pyrazoles, triazoles, pyrimidines, pyrazines, thiazoles, isoxazoles, isothiazoles, tetrazoles, or oxadiazoles) and heteroaryl ring systems in which a carbocyclic aromatic ring, carbocyclic non-aromatic ring or heteroaryl ring is fused to one or more other heteroaryl rings (e.g., benzo(b)thienyl, benzimidazole, indole, tetrahydroindole, azaindole, indazole, quinoline, imidazopyridine, purine, pyrrolo[2,3-d]pyrimidine, pyrazolo[3,4-d]pyrimidine) and their N-oxides.

An aralkyl group, as used herein, is an aromatic substituent that is linked to a compound by an aliphatic group having from one to about six carbon atoms.

An heteroaralkyl group, as used herein, is a heteroaromatic substituent that is linked to a compound by an aliphatic group having from one to about six carbon atoms.

A heterocycloalkyl group, as used herein, is a non-aromatic ring system that has 3 to 8 atoms and includes at least one heteroatom, such as nitrogen, oxygen, or sulfur.

An acyl group, as used herein, is an $-C(O)NR_xR_z$, $-C(O)OR_x$, $-C(O)R_x$, in which R_x and R_z are each, independently, -H, a substituted or unsubstituted aliphatic group or a substituted or unsubstituted aromatic group.

As used herein, aliphatic groups include straight chained, branched or cyclic C_1 - C_8 hydrocarbons which are completely saturated or which contain one or more units of unsaturation. A "lower alkyl group" is a saturated aliphatic group having form 1-6 carbon atoms.

Inhibitor I bound to the catalytically inactive mutant of Tie-2 (see Fig. 2 for sequence and Fig. 3 for atomic coordinates) crystallized in the space group C2221. The x-ray crystallographic structure revealed the following interactions:

The pyrrolopyrimidine ring of the inhibitor I forms hydrogen bonds to residues in the hinge region and interacts with purine core region. The core of the inhibitor presents a hydrogen bond donor in the form of the amino proton of the 4-NH₂

substituent to the carbonyl oxygen of E903. Atom N3 of the pyrimidine ring accepts a hydrogen bond from the backbone N-H of A905. The ring system of the core presents a planar face to residues of both the C-terminal and N-terminal lobes. The residues in these areas present a hydrophobic surface which "sandwiches" the planar core of the inhibitor. Residues involved in this hydrophobic sandwich region include I830, V838, I86, I902 and L971. Atoms N1 and N7 of the core face the solvent exposed mouth of the binding pocket. Atom C6 faces the long axis of the nucleotide binding loop of the N-terminal lobe of the protein.

The N7 cyclopentane ring is directed towards solvent but is still within the protein cavity. This region was described above as the extended sugar pocket after the binding mode of the ribose ring of ATP observed in other kinase structures. This region is characterized by hydrophobic interactions with primarily I830 and L971. Methylene groups of E832 may also contribute in this fashion.

The phenyl ring attached to C5 of the pyrrolopyrimidine ring is in a predominantly hydrophobic area, generated by residues from the purine core region, the distal hydrophobic pocket and methylene groups from the catalytic lysine, K855. The hydrophobic contacts are with residues V838, I886, I902, L971 and A981. Lysine 855 is highly mobile, so it is also possible that the Cl atom meta to the pyrrolopyrimidine ring is receiving a hydrogen bond.

The sulfonamide linker makes a clear hydrogen bond with an amide proton of D982 and may also make a hydrogen bond to the amide proton of F983.

The terminal phenyl ring (labelled ring C) is located in the distal hydrophobic pocket. Primary contacts are with L876, I886, L888 and F983.

Inhibitor II bound to the catalytically inactive mutant of Tie-2 (see Fig. 2 for sequence and Fig. 4 for atomic coordinates) crystallized in the space group P42212. The x-ray crystallographic structure revealed the following additional interactions:

The pyrrolopyrimidine core, B-ring, linker and C-ring bind the same way as inhibitor I. The N-7 cyclohexyl N-methyl piperazinyl group occupies the extended sugar pocket and makes a strong ionic interaction with D912.

Inhibitor III bound to the catalytically inactive mutant of Tie-2 (see Fig. 2 for sequence and Fig. 4 for atomic coordinates) crystallized in the space group P42212.

The x-ray crystallographic structure revealed the following additional interactions:

5 The pyrrolopyrimidine core binds the same way as inhibitor I. The N-7 cyclohexyl N-methy piperazinyl group occupies the extended sugar pocket and makes a strong ionic interaction with D912 as in Tie-2/inhibitor II. The B-ring binds in a similar fashion to inhibitor I, however, the hydrogen bond between a halogen, fluorine in this case, and K855 is more clear. The linker makes two clear hydrogen bonds to backbone amide protons of D983 and F983. The C-ring occupies the distal hydrophobic pocket with main interactions coming from L876, I886, L888, L900, I902 and F983.

10 Inhibitor IV bound to the catalytically inactive mutant of Tie-2 (see Fig. 2 for sequence and Fig. 4 for atomic coordinates) crystallized in the space group P42212. The x-ray crystallographic structure revealed the following additional interactions:

15 The pyrrolopyrimidine core binds the same way as inhibitor I. The N-7 cyclohexyl N-methy piperazinyl group occupies the extended sugar pocket and makes a strong ionic interaction with D912 as in Tie-2/inhibitor II. The B-ring binds in a similar fashion to inhibitor I, however there is no chlorine atom to act as a potential hydrogen bond partner. The linker in this case is an oxygen atom which accepts a hydrogen bond from the catalytic lysine, K855. The C-ring occupies the distal hydrophobic pocket with main interactions coming from L876, I886, I902 and F983.

20 In one embodiment, the present invention relates to a method of treating a Tie-2-dependent condition in a patient. The method comprises the step of administering to the patient a therapeutically effective amount of a Tie-2 inhibitor as described above. The patient can be any animal, and is, preferably, a mammal and, more preferably, a human.

25 A "Tie-2-dependent condition" is a disease or medical condition in which the catalytic activity of Tie-2 plays a role, for example, in the development of the disease or condition. For example, in one embodiment, the condition is characterized by excessive vascular proliferation. Tie-2 inhibitors are useful in treating angiogenesis dependent disorders, and disorders involving aberrant endothelial-pereendothelial interactions (e.g., restenosis).

30

Tie-2 dependent conditions include hyperproliferative disorders, cancer, a cardiovascular condition, an ocular condition, von Hippel Lindau disease, pemphigoid, psoriasis, Paget's disease, polycystic kidney disease, fibrosis, sarcoidosis, cirrhosis, thyroiditis, Osler-Weber-Rendu disease, chronic inflammation, synovitis, inflammatory bowel disease, Crohn's disease, rheumatoid arthritis, osteoarthritis, psoriatic arthritis, an ulcer and sepsis. In addition a Tie-2 inhibitor can be used to decrease fertility in a patient.

Preferred methods of treatment are where the cancer is a solid tumor, a sarcoma, fibrosarcoma, osteoma, melanoma, retinoblastoma, a rhabdomyosarcoma, glioblastoma, neuroblastoma, teratocarcinoma, an hematopoietic malignancy, malignant ascites, Kaposi's sarcoma, Hodgkin's disease, lymphoma, myeloma or leukemia.

Another preferred method of treatment is where the cardiovascular condition, atherosclerosis, restenosis, ischemia/reperfusion injury, chronic occlusive pulmonary disease, vascular occlusion, carotid obstructive disease, Crow-Fukase (POEMS) syndrome, anemia, ischemia, infarct, vascular leakage disorders.

Yet another preferred method of treatment is where the ocular condition is ocular or macular edema, ocular neovascular disease, scleritis, radial keratotomy, uveitis, vitritis, myopia, optic pits, chronic retinal detachment, post-laser treatment complications, conjunctivitis, Stargardt's disease, Eales disease, retinopathy, macular degeneration or microangiopathy.

A Tie-2 inhibitor can also be used in a method of promoting angiogenesis or vasculogenesis. In addition, a Tie-2 inhibitor can be administered with a pro-angiogenic growth factor.

A therapeutically effective amount, as this term is used herein, is an amount which results in partial or complete inhibition of disease progression or symptoms. Such an amount will depend, for example, on the size and gender of the patient, the condition to be treated, the severity of the symptoms and the result sought, and can be determined by one skilled in the art.

The compound of the invention can, optionally, be administered in combination with one or more additional drugs or therapies which, for example, are

known for treating and/or alleviating symptoms of the condition mediated by Tie-2. The additional drug can be administered simultaneously with the compound of the invention, or sequentially. For example, the Tie-2 inhibitor can be administered in combination with another anticancer agent, as is known in the art. Additional
5 therapies which may be coadministered would include, for example, radiation therapy, ultraviolet irradiation, hyperthermia, laser irradiation, targeted radionuclides and neutron bombardment.

The invention further provides pharmaceutical compositions comprising one or more of the Tie-2 inhibitors described above. Such compositions comprise a
10 therapeutically (or prophylactically) effective amount of one or more Tie-2 binding inhibitors, as described above, and a pharmaceutically acceptable carrier or excipient.

Suitable pharmaceutically acceptable carriers include, but are not limited to, saline, buffered saline, dextrose, water, glycerol, ethanol, and combinations thereof. The carrier and composition can be sterile. The formulation should suit the mode of
15 administration.

Suitable pharmaceutically acceptable carriers include but are not limited to water, salt solutions (e.g., NaCl), alcohols, gum arabic, vegetable oils, benzyl alcohols, polyethylene glycols, gelatin, carbohydrates such as lactose, amylose or starch, cyclodextrin, magnesium stearate, talc, silicic acid, viscous paraffin, perfume
20 oil, fatty acid esters, hydroxymethylcellulose, polyvinyl pyrrolidone, etc. The pharmaceutical preparations can be sterilized and if desired, mixed with auxiliary agents, e.g., lubricants, preservatives, stabilizers, wetting agents, emulsifiers, salts for influencing osmotic pressure, buffers, coloring, flavoring and/or aromatic substances and the like which do not deleteriously react with the active compounds.

The composition, if desired, can also contain minor amounts of wetting or emulsifying agents, or pH buffering agents. The composition can be a liquid solution, suspension, emulsion, tablet, pill, capsule, sustained release formulation, or powder. The composition can be formulated as a suppository, with traditional binders and carriers such as triglycerides. Oral formulation can include standard carriers such as
30 pharmaceutical grades of mannitol, lactose, starch, magnesium stearate, polyvinyl pyrrolidinone, sodium saccharine, cellulose, magnesium carbonate, etc.

The composition can be formulated in accordance with the routine procedures as a pharmaceutical composition adapted for intravenous administration to human beings. Typically, compositions for intravenous administration are solutions in sterile isotonic aqueous buffer. Where necessary, the composition may also include a solubilizing agent and a local anesthetic to ease pain at the site of the injection. Generally, the ingredients are supplied either separately or mixed together in unit dosage form, for example, as a dry lyophilized powder or water free concentrate in a hermetically sealed container such as an ampoule or sachet indicating the quantity of active agent. Where the composition is to be administered by infusion, it can be dispensed with an infusion bottle containing sterile pharmaceutical grade water, saline or dextrose/water. Where the composition is administered by injection, an ampoule of sterile water for injection or saline can be provided so that the ingredients may be mixed prior to administration.

The pharmaceutical compositions of the invention can also include an agent which controls release of the Tie-2 inhibitor compound, thereby providing a timed or sustained release composition.

The Tie-2 inhibitor can be administered subcutaneously, intravenously, parenterally, intraperitoneally, intradermally, intramuscularly, intraocularly, topically, enteral (e.g., orally), rectally, nasally, buccally, sublingually, vaginally, by inhalation spray, by drug pump or via an implanted reservoir in dosage formulations containing conventional non-toxic, physiologically acceptable carriers or vehicles. The preferred method of administration is by oral delivery. The form in which it is administered (e.g., syrup, elixir, capsule, tablet, solution, foams, emulsion, gel, sol) will depend in part on the route by which it is administered. For example, for mucosal (e.g., oral mucosa, rectal, ocular mucosa, intestinal mucosa, bronchial mucosa) administration, nose drops, aerosols, inhalants, nebulizers, eye drops or suppositories can be used. The compounds and agents of this invention can be administered together with other biologically active agents, such as analgesics, anti-inflammatory agents, anesthetics and other agents which can control one or more symptoms or causes of a Tie-2 dependent condition.

In a specific embodiment, it may be desirable to administer the agents of the invention locally to a localized area in need of treatment; this may be achieved by, for example, and not by way of limitation, local infusion during surgery, topical application, transdermal patches, by injection, by means of a catheter, by means of a suppository, or by means of an implant, said implant being of a porous, non-porous, or gelatinous material, including membranes, such as sialastic membranes or fibers. For example, the agent can be injected into the joints.

EXAMPLES

10

Example 1 Protein Purification

(His)₆Tie-2 802-1124, D964N, which contains a TEV protease cleavage peptide, was expressed recombinantly by baculovirus infection of SF-9 cells. Cells were lysed in a buffer containing 20 mM Tris pH 8.0, 137 mM NaCl, 10 % glycerol, 1 % Triton X-100, 1 mM ADP, 5 mM MgCl₂ and complete protease inhibitor, EDTA-free cocktail from Boehringer Mannheim.. The ligand ADP/Mg⁺⁺ was maintained at this concentration in buffers of all subsequent purification steps. The cell lysate was centrifuged and the supernatant was applied to a Ni⁺⁺ chelating sepharose column which had been equilibrated in 50 mM HEPES, pH 7.5, 0.3 M NaCl. Tie-2 was eluted by competition with 100 mM imidazole. The eluted (His)₆ Tie-2 was digested with Tev protease and dialyzed against 50 mM HEPES, pH 7.5, 0.25 M NaCl, 5 mM DTT. The dialyzed sample was centrifuged to remove any precipitated protein, and Tie-2 was bound to a MonoQ anion exchange column and eluted with a linear 20 column volume gradient of 0.025-0.2 M NaCl. Typically, differences in the monodispersity of early eluting verses late eluting fractions could be detected using Dynamic Light Scattering (DLS). Sample purity was assessed with SDS-PAGE, native PAGE, and LC/MS total mass analysis. Fractions with similar DLS characteristics were pooled and concentrated to greater than 2 mg/ml using ultrafiltration at -80 °C. The ultracentrifuged samples were used in crystallographic

experiments described below. Table I lists a range of conditions suitable for crystallization.

Example 2:

5

I. Diphosphorylated Tie-2 802-1124

A. Crystallization Conditions:

10 Tie-2 802-1124 (2PO₄) protein was crystallized in a sitting or hanging drop geometry using a vapor diffusion method. The protein concentration was 5 mg/ml, and the well solution was 10% PEG 6,000; 0.1 M HEPES, pH 7.5; 5% MPD (2-methyl-2,4-pentanediol). Drops were set up using equal volumes of protein and well solution containing 500 μM inhibitor. Crystals routinely grew to 0.4 mm x 0.1 mm x 0.01 mm in about a week. Crystals were of the space group P2(1)2(1)2(1) with unit
15 cell dimensions $a = 54.320 \text{ \AA}$, $b = 75.872 \text{ \AA}$, $c = 78.143 \text{ \AA}$, and $\alpha = \beta = \gamma = 90.0^\circ$. Table I list a range of conditions which are suitable for crystallization.

B. Data Collection

20 Data on ligand bound crystals were collected on a Rigaku RU300 rotating anode generator running at 50kV 150 mA equipped with an R-Axis II phosphoimage plate detector. X-rays were monochromatized by long mirrors and filtered with a 0.0067μm Nickel filter. Data were processed and reduced with DENZO and SCALEPACK (Minor, W. 1993). Data were collected to 3.5 Å resolution.

25 C. Data Processing

Programs in the CCP4 suite (Collaborative Computational Project, Number 4 1994) (tomtz, trunc, cad and ecalc) were used to format and process the data for molecular replacement. The molecular replacement program AMORE (Navaza, J. 1994) was used successfully to find phases for the data set using an initial model. The
30 initial model was composed of the carboxy-terminal portion (residues 566-575 and 592-672) of the FGFR kinase domain trimmed back to poly-Alanine (PDB accession number 1FGK). A second round of AMORE with a more complete model (residues

464-485, 491-500, 505-575 and 592-762) was also performed to confirm the phasing solution.

D. Optimization of Model

5 Several round of least-squared minimization using CNS (Brunger, A.T. et al., 1998) alternating with manual rebuilding, using the graphics program O, version 6.2.1 (Jones, A., 1997; Kleywegt G. J., 1995) were performed iteratively to improve the model while comparing it to electron density maps generated after each round with coefficients 2fo-fc contoured at a level of 1.0 sigma.

10

II. Tie-2 (D964N) 802-1124 (SEQ ID NO 2)

A. Crystallization Conditions

Purified Tie-2 (D964N) 802-1124 protein was crystallized in a sitting drop
15 geometry using the vapor diffusion method. The protein concentration was 2.5 mg/ml, and the well solution was 1.0 to 1.5 M ammonium sulfate, 0.1M MES, pH 6.5, 5% dioxane (1,4-dioxane). Drops were set up using equal volumes of protein and well solution containing 100-300 μ M inhibitor. Crystals routinely grew to 0.3 mm x 0.05 mm x 0.01 mm in about 2-3 days. Crystals of Tie-2/inhibitor I were of the space
20 group C222(1) with unit cell dimensions $a = 75.195 \text{ \AA}$, $b = 116.287 \text{ \AA}$, $c = 95.060 \text{ \AA}$ and $\alpha = \beta = \gamma = 90.0^\circ$. Crystals of the Tie-2/inhibitor II, III or IV complex were of the space group P42212 with unit cell dimensions $a = b = 86.0 \text{ \AA}$, $c = 112.0 \text{ \AA}$ and $\alpha = \beta = \gamma = 90.0^\circ$.

25 B. Data Collection

Data on a ligand-bound crystal (Tie-2 (D964N) 802-1124) complexed with inhibitors I, II, III, or IV were collected at the beamline X25 at Brookhaven National Laboratory (Upton, NY) equipped with the Brandeis B4, CCD detector. Data were processed and reduced with DENZO and SCALEPACK (Minor, W. 1993). Data for
30 the Tie-2/inhibitor I complex were collected complete to 2.75 \AA resolution, with higher resolution reflections visible to 2.0 \AA resolution.

C. Data Processing

Programs in the CCP4 suite (Collaborative Computational Project, Number 4 1994) (tomtz, trunc, cad and ecalc) were used to format and process the data for molecular replacement. The molecular replacement program AMORE (Navaza, J. 5 1994) was used successfully to find phases for the data set using an initial model. The initial model was composed of the a conservative portion of the FGFR kinase domain (Tie2 residue numbering 818-830, 841-842, 850-857, 866-890, 900-916, 935-981, 1001-1093). The model, mostly poly-Alanine, was trimmed of loop regions which diverged upon superposition of five tyrosine kinase structures (IRK, HCK, SRC, 10 FGFR, and LCK). In addition this model included only those side-chain residues in positions where an identical side-chain was found in the FGFR model.

D. Optimization of Model

Several round of least-squared minimization using CNS (Brunger, A. T. et al., 15 1998) alternating with manual rebuilding, using the graphics program O, version 6.2 (Jones, A., 1997; Kleywegt G. J., 1995) were performed to iteratively improve the model while comparing it to two electron density maps: one generated with coefficients 2fo-fc contoured at a level of 1.0 sigma and the other generated with coefficients fo-fc contoured at a level of 1.5 sigma.

20

E. Inhibitor Docking

Inhibitor I was found to be bound to the active site. It was initially docked by hand in O by visually inspecting the electron density maps and adjusting the torsion angles of the inhibitor. Parameter and topology files were generated for CNS using 25 the X-util program xplo2d (Kleywegt G. J. and Jones, T.A. 1997) and modified slightly to properly model chlorine in the inhibitor.

III. Tie-2 (D964N) 802-1124 (SEQ ID NO 2)

A. Crystallization Conditions

5 The protein (construct Tie-2D964N) was provided in a buffer containing 25mM HEPES, pH 7.5, 50 mM NaCl, 5 mM MgCl₂, 1 mM ADP and 5 mM DTT. The protein concentration was about 2.3 mg/ml as determined with a Coomassie Plus assay, BSA as standard.

10 The inhibitor III was dissolved in DMSO to give a 50 mM stock solution. Stock solution was added to the protein solution for a final inhibitor concentration of 2mM. Crystallization conditions were screened with Hampton Screen *Crystal screen*, *Crystal screen2*, *Membfac*, *Natrix* and *PEG/ion screen* at room temperature and 4°C. Crystals grew with precipitation buffer: 20% PEG 3350, 0,2M tri-Lithium Citrat pH 8,1 (Hampton Screen *PEG/ion screen*, Nr. 45) sitting or hanging drop: 750µl buffer in
15 reservoir in the drop typically 1µl - 2µl protein and 1µl - 2µl reservoir solution were mixed.

Addition of the following additives (10% by volume to the drop) also yielded crystals:

Add. Screen I Nr.:01	0.1M Ba-Chloride
Add. Screen I Nr.:03	0.1M Ca-Chloride
Add. Screen I Nr.:06	0.1M Mg-Chloride
Add. Screen I Nr.:16	0.1M Trimehylamine
Add. Screen I Nr.:22	30% Ethanol
Add. Screen II Nr.:08	30% Xylitol
Add. Screen II Nr.:13	30% 1,5Diaminopentan-dihydrochloride
Add. Screen II Nr.:14	30% 1,8 Diaminooctane
Add. Screen II Nr.:17	0.1M Hexaaminocobalt-trichloride
Add. Screen III Nr.:02	1.0M Cesium-chloride

Add. Screen III Nr.:04	1.0M Lihium-chloride
Add. Screen III Nr.:06	0.5M Sodium-flouride
Add. Screen III Nr.:16	40% Acetonitrile
Add. Screen III Nr.:18	40% n-Propanol
Add. Screen III Nr.:19	5% Ethyl-acetate
Add. Screen III Nr.:20	40% Acetone
Add. Screen III Nr.:21	2,5% Dichlormethane
Add. Screen III Nr.:22	7% n-Butanol
Add. Screen III Nr.:24	0.1M 1,4 Dithio-DL-threitol

B. Data collection:

Data were measured at the beam line BW 6 of the Max-Planck-Society at DESY, Hamburg.

5 The crystals were shock cooled to 100 K; cryobuffer was crystallization buffer plus 20 – 30 % glycerol. 213 frames with $\Delta\phi=0.25$ degrees were collected with a MAR CCD detector, at a crystal detector distance of 120mm and a wavelength of 1.072Å.

10 Crystals are of a tetragonal space group with unit cell dimensions $a=b=86.0$ Å and $c=112.0$ Å. The cell dimensions of different crystals vary (for a and b between 85 and 87Å, for c between 97 and 113). Extinctions indicate the space group P42212 which was confirmed by molecular replacement.

Table II: Crystallization conditions for Tie-2/inhibitor complexes.

Condition	Tie-2 802-1124 D964N	Tie-2 802-1124 (diphosphorylated)
<i>Protein concentration</i>	2.5 mg/mL optimal range 1.5 – 4 mg/mL limits 1.0 – 5.0 mg/mL	5 mg/mL optimal range 2.5 – 10 mg/mL
<i>Buffer concentration</i>	100 mM MES optimal range 50–250 mM Limits 20–300 mM	100 mM HEPES optimal Range 50-150 mM Limits 20-300 mM
<i>pH</i>	6.5 optimal range 5.5 – 7.5	7.5 optimal range 7.0 – 7.7 limits 6.5 – 8.0
<i>Buffer Identity</i>	Buffers capable of buffering in a similar pH range expected to give similar results	(same)
<i>Precipitant</i>	(NH ₄) ₂ SO ₄ Range 1.0 – 1.5 M Limits 0.7 – 1.8 M	10% PEG 6000 optimal conc. range 5-15% conc. limits 1 – 20% MW range 4000 – 8000 MW limits may be much wide
<i>Additive parameters</i>	5% 1,4-dioxane optimal range 0 – 10% (higher concentrations etch the plastic vessel in which the experiment is done; higher concentrations may be possible in a resistant vessel) 1,3-dioxane, similar molecules, or mixtures in various ratios should also give similar results	5% MPD (2-Me-2,4-pentanediol) optimal range 0 – 10%

<i>Additive identities</i>	<p>Examples which have been successfully added:</p> <p>1,5-diaminopentane</p> <p>Glycerol (1-10%)</p> <p>Ethylene glycol (1-10%)</p> <p>Spermidine (10 – 300 mM)</p> <p>Combinations, in varying ratios, may give similar results</p>	(same)
<i>Drop volumes and ratios</i>	<p>2 μL protein + 2 μL well solution optimal</p> <p>Total volume range: up to 200 μL, assuming a sitting geometry for larger volumes</p> <p>Volume Ratio range: 1 part protein to 0.5 – 2.0 parts well solution</p>	(same)
<i>Well volume (for 4 μL crystallization drop)</i>	<p>Range 500 – 1000 μL</p> <p>Limits 250 – large volume (limited by the distance between the drop and the surface of the well solution allowed by the vessel geometry, see below)</p>	(same)
<i>Drop – well solution distance</i>	<p>2 cm optimal</p> <p>Range 1-4 cm</p> <p>Limits: 0.1 cm - 5 cm</p>	(same)
<i>Temperature</i>	<p>room temp optimal (22 – 25 °C)</p> <p>limits 17 – 30 °C</p>	(same)
<i>Ligands</i>	<p>ADP/Mg²⁺ and analogs</p> <p>Inhibitors: inhibitors I-IV, analogs</p> <p>Expect similar results from ligands that bind reversibly under crystallization conditions with K_d values < 1 mM</p>	(same)

<i>Constructs</i>	<p>Variants in amino acid sequence that crystallize in the same space group and unit cell should be considered equivalent</p> <p>Additional constructs would include deletion of unstructured termini as determined by crystal structure of this construct. For example, deletion of the C-terminal 24 residues (leaving 802-1100) has been prepared, which is likely to yield similar results</p>	(same)
<i>Posttranslational modification</i>	Variants in posttranslational modification that crystallize in the same space group and unit cell should be considered equivalent	<p>2 phosphate forms have been crystallized. This protein contains one phosphate on either Y897 or Y899 and one on one of five T residues, at amino acids 1012, 1024, 1040, and 1048</p> <p>Other phosphorylated forms may give similar results.</p> <p>A single phosphate species has been observed in which the phosphate is on either Y897 or Y899 and has also been isolated.</p> <p>In addition, 3 and 4 phosphate species have been isolated which may crystallize.</p>
<i>Space group</i>	C222(1)	P2(1)2(1)2(1)
<i>Unit cell</i>	<p>$a = 75.195 \text{ \AA}$, $b = 116.287 \text{ \AA}$, $c = 95.060 \text{ \AA}$</p> <p>Variations of $\pm 2\%$ should be considered equivalent</p> <p>Angles: $a = b = c = 90^\circ$</p> <p>Observed variations of $\pm 1\%$ should be considered equivalent</p>	<p>$a = 54.320 \text{ \AA}$, $b = 75.872 \text{ \AA}$, $c = 78.143 \text{ \AA}$</p> <p>Variations of $\pm 2\%$ should be considered equivalent</p> <p>Angles: $a = b = c = 90^\circ$</p> <p>Observed variations of $\pm 1\%$ should be considered equivalent</p>

<i>Other crystallization tricks that should give at least equivalent results</i>	Low gravity Temperature oscillations Presence of cryoprotectant (15-25% glycerol added before data collection) Variations in crystallization tray geometry Data collection temperature (range: minus 180 to plus 25 °C)	(same)
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REFERENCES:

- 5 Brunger, A.T., Adams, P. D., Clore, G. M., DeLano, W. L. Gros, P. Grosse-Kunstleve, R. W., Jiang, J-S., Kuszewski, J., Nigels, M., Pannu, N. S., Read, R. J., Rice, L. M., Simonson, T., and Warren, G. L.. (1998) *Acta Cryst.*, *D54*, 905-921.
- 10 Collaborative Computational Project, Number 4 (1994) The CCP4 Suite: Programs for Protein Crystallography. *Acta Cryst.* *D50*, 760-763.
- Jones, A.T and Kjeldgaard, M. (1997) *Methods in Enzymology* 277, 173-208.
- 15 Kleywegt G. J. and Jones, T.A. (1997) *Methods in Enzymology* 277, 525-545.
- Kleywegt G. J., (1995) *ESF/CCP4 Newsletter* 31, 45-50.
- Minor, W. XDISPLAYF program, Purdue University (1993)
- 20 Navaza, J. (1994) *Acta Cryst.* *A50*, 157-163.

Example 3: *In Vitro* Potency Test of Tie-2 Inhibitors

The *in vitro* potency of compounds in inhibiting these protein kinases may be determined by the procedures detailed below.

5 The potency of compounds can be determined by the amount of inhibition of the phosphorylation of an exogenous substrate (e.g., synthetic peptide (Z. Songyang *et al.*, *Nature*. 373:536-539) by a test compound relative to control.

Human Tie-2 Kinase Production and Purification

10 The coding sequence for the human Tie-2 intra-cellular domain (aa775-1124) was generated through PCR using cDNAs isolated from human placenta as a template. A poly-His₆ sequence was introduced at the N-terminus and this construct was cloned into transfection vector pVL 1939 at the Xba 1 and Not 1 site. Recombinant BV was generated through co-transfection using the BaculoGold Transfection reagent (PharMingen). Recombinant BV was plaque purified and verified through Western
15 analysis. For protein production, SF-9 insect cells were grown in SF-900-II medium at 2 x 10⁶/ml, and were infected at MOI of 0.5. Purification of the His-tagged kinase used in screening was analogous to that described for KDR.

EGFR Tyrosine Kinase Source

20 EGFR was purchased from Sigma (Cat # E-3641; 500 units/50 μ l) and the EGF ligand was acquired from Oncogene Research Products/Calbiochem (Cat # PF011-100).

Enzyme Linked Immunosorbent Assay (ELISA) For PTKs

Enzyme linked immunosorbent assays (ELISA) were used to detect and measure the presence of tyrosine kinase activity. The ELISA were conducted
25 according to known protocols which are described in, for example, Voller, *et al.*, 1980, "Enzyme-Linked Immunosorbent Assay," In: *Manual of Clinical Immunology*, 2d ed., edited by Rose and Friedman, pp 359-371 Am. Soc. of Microbiology, Washington, D.C.

30 The disclosed protocol was adapted for determining activity with respect to a specific PTK. For example, preferred protocols for conducting the ELISA experiments is provided below. Adaptation of these protocols for determining a

compound's activity for other members of the receptor PTK family, as well as non-receptor tyrosine kinases, are well within the abilities of those skilled in the art. For purposes of determining inhibitor selectivity, a universal PTK substrate (e.g., random copolymer of poly(Glu₄ Tyr), 20,000-50,000 MW) was employed together with ATP
5 (typically 5 μ M) at concentrations approximately twice the apparent K_m in the assay.

The following procedure was used to assay the inhibitory effect of compounds of this invention on Tie-2 tyrosine kinase activity:

Buffers and Solutions:

10 PGTPoly (Glu,Tyr) 4:1

Store powder at -20°C. Dissolve powder in phosphate buffered saline (PBS) for 50mg/ml solution. Store 1ml aliquots at -20°C. When making plates dilute to 250 μ g/ml in Gibco PBS.

Reaction Buffer: 100mM Hepes, 20mM MgCl₂, 4mM MnCl₂, 5mM DTT,
15 0.02%BSA, 200 μ M NaVO₄, pH 7.10

ATP: Store aliquots of 100mM at -20°C. Dilute to 20 μ M in water

Washing Buffer: PBS with 0.1% Tween 20

Antibody Diluting Buffer: 0.1% bovine serum albumin (BSA) in PBS

TMB Substrate: mix TMB substrate and Peroxide solutions 9:1 just before use or use

20 K-Blue Substrate from Neogen

Stop Solution: 1M Phosphoric Acid

Procedure

1. Plate Preparation:

25 Dilute PGT stock (50mg/ml, frozen) in PBS to a 250 μ g/ml. Add 125 μ l per well of Corning modified flat bottom high affinity ELISA plates (Corning #25805-96). Add 125 μ l PBS to blank wells. Cover with sealing tape and incubate overnight 37°C. Wash 1x with 250 μ l washing buffer and dry for about 2hrs in 37°C dry incubator. Store coated plates in sealed bag at 4°C until used.

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2. Tyrosine Kinase Reaction:

-Prepare inhibitor solutions at a 4x concentration in 20% DMSO in water.

-Prepare reaction buffer

5 -Prepare enzyme solution so that desired units are in 50 μ l, e.g. for KDR make to 1 ng/ μ l for a total of 50ng per well in the reactions. Store on ice.

-Make 4x ATP solution to 20 μ M from 100mM stock in water. Store on ice

-Add 50 μ l of the enzyme solution per well (typically 5-50 ng enzyme/well depending on the specific activity of the kinase)

10 -Add 25 μ l 4x inhibitor

-Add 25 μ l 4x ATP for inhibitor assay

-Incubate for 10 minutes at room temperature

-Stop reaction by adding 50 μ l 0.05N HCl per well

-Wash plate

15 **Final Concentrations for Reaction: 5 μ M ATP, 5% DMSO

3. Antibody Binding

-Dilute 1mg/ml aliquot of PY20-HRP (Pierce) antibody (a phosphotyrosine antibody) to 50ng/ml in 0.1% BSA in PBS by a 2 step dilution (100x, then 200x)

20 -Add 100 μ l Ab per well. Incubate 1 hr at room temp. Incubate 1 hr at 4C.

-Wash 4x plate

4. Color reaction

-Prepare TMB substrate and add 100 μ l per well

25 -Monitor OD at 650nm until 0.6 is reached

-Stop with 1M Phosphoric acid. Shake on plate reader.

-Read OD immediately at 450nm

Optimal incubation times and enzyme reaction conditions vary slightly with enzyme preparations and are determined empirically for each lot.

Example 4: Cellular Assay for Determining the Potency of Tie-2 Inhibitors

The following cellular assay can be used to determine the potency of a Tie-2 inhibitor.

5 "NIH-3T3/hTEK Cell line:

A retroviral expression vector containing the full length Tie-2 cDNA, LNCX6 h-TEK, was kindly provided to us by Dr. Kevin Peters. A tumorigenic subline of NIH 3T3 cells was transfected with 10 μ g of LNCX6 h-TEK by calcium phosphate precipitation method and selected with 400 μ g/ml neomycin. Individual clones were isolated and
10 analyzed for the presence of Tie-2 protein by Western blotting. Maximum expression of Tie-2 was observed in clone #67. Expression of Angiopoietin 1 message has been shown using PCR and an autocrine loop is revealed in the presence of vanadate

Cellular Tie-2 assay:

15 Tie-2 cellular autophosphorylation was measured using the NIH-3T3/hTEK (hTEK) cell line. Cells were seeded in 96 well plates overnight. The media was removed and cells treated with inhibitor for 20 minutes and phosphatase inhibitor NaVO_3 (2mM) for 15 more minutes. Cells were lysed with RIPA buffer and lysates were immunoprecipitated using a specific α -Tie-2 monoclonal antibody (KP33,
20 provided by Dr. Kevin Peters) and the IP'd protein run on SDS PAGE. The phosphotyrosine level on Tie2 protein were then determined by α -phosphotyrosine antibodies (4G10, Upstate Biotechnology) on Western blots. Films were scanned and % inhibition as compared to untreated control was determined."

25 EQUIVALENTS

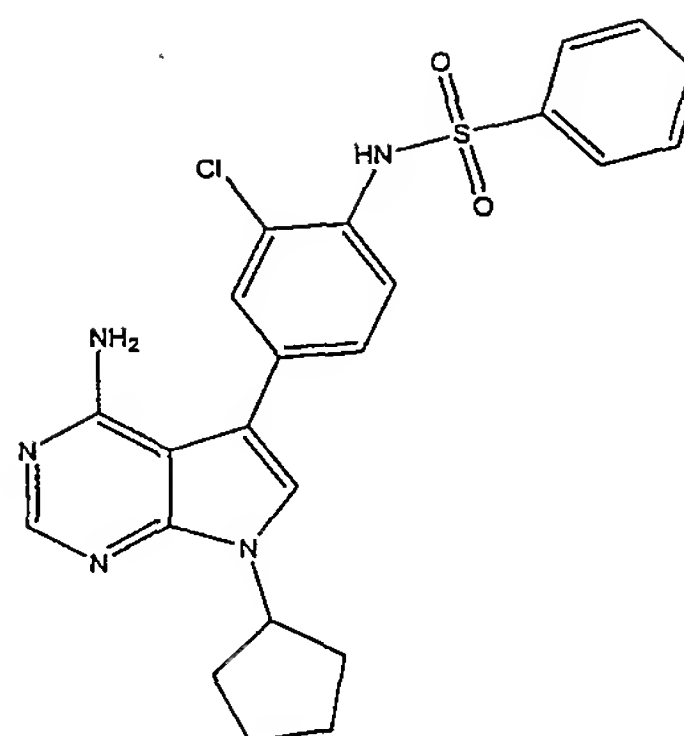
While this invention has been particularly shown and described with references to preferred embodiments thereof, it will be understood by those skilled in the art that various changes in form and details may be made therein without departing from the scope of the invention encompassed by the appended claims.

CLAIMS

What is claimed is:

1. A crystalline polypeptide, said polypeptide comprising the catalytic domain of
5 a Tie-2 protein.
2. The crystalline polypeptide of Claim 1 wherein the polypeptide comprises the catalytic domain of human Tie-2.
- 10 3. A crystalline polypeptide-ligand complex, said polypeptide comprising the catalytic domain of a Tie-2 protein.
4. The crystalline polypeptide/ligand complex of Claim 3 wherein the polypeptide comprises the catalytic domain of a mammalian Tie-2.
- 15 5. The crystalline polypeptide/ligand complex of Claim 4 wherein the mammalian Tie-2 protein is human Tie-2.
6. The crystalline polypeptide/ligand complex of Claim 5 wherein the
20 polypeptide comprises amino acids 802-1124 of SEQ ID NO: 1.
7. The crystalline polypeptide/ligand complex of Claim 6 wherein the ligand is of the formula:

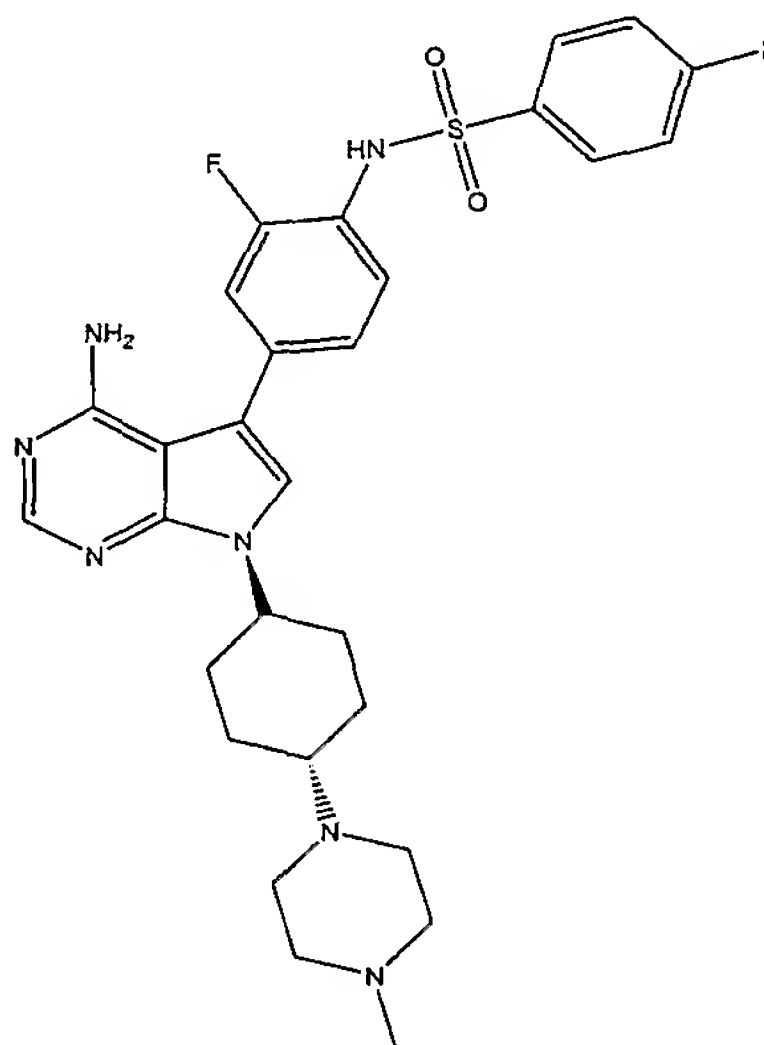
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8. The crystalline polypeptide/ligand complex of Claim 7 having unit cell parameters a is about 96 Å, b is about 118 Å, c is about 78 Å and $\alpha = \beta = \gamma = 90^\circ$.

9. The crystalline polypeptide/ligand complex of Claim 6 wherein the ligand is of the formula:

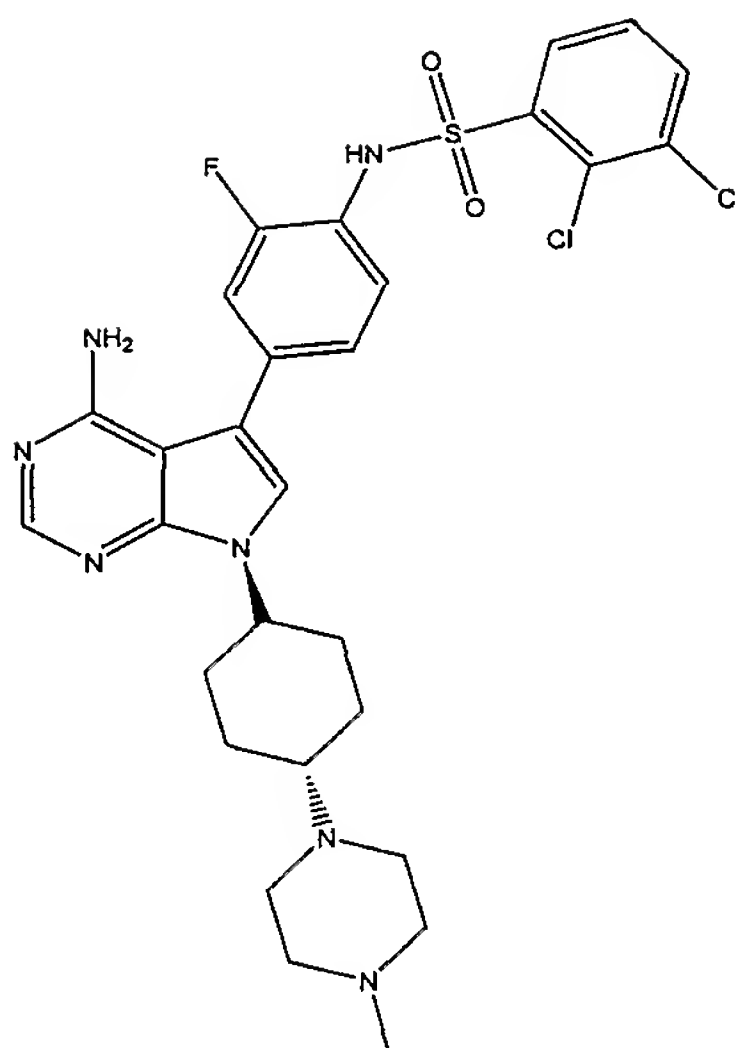


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10. The crystalline polypeptide/ligand complex of Claim 9 having unit cell parameters a and b are about 86.0 Å, c is about 112.0 Å and $\alpha = \beta = \gamma = 90^\circ$.

11. The crystalline polypeptide/ligand complex of Claim 6 wherein the ligand is of the formula:

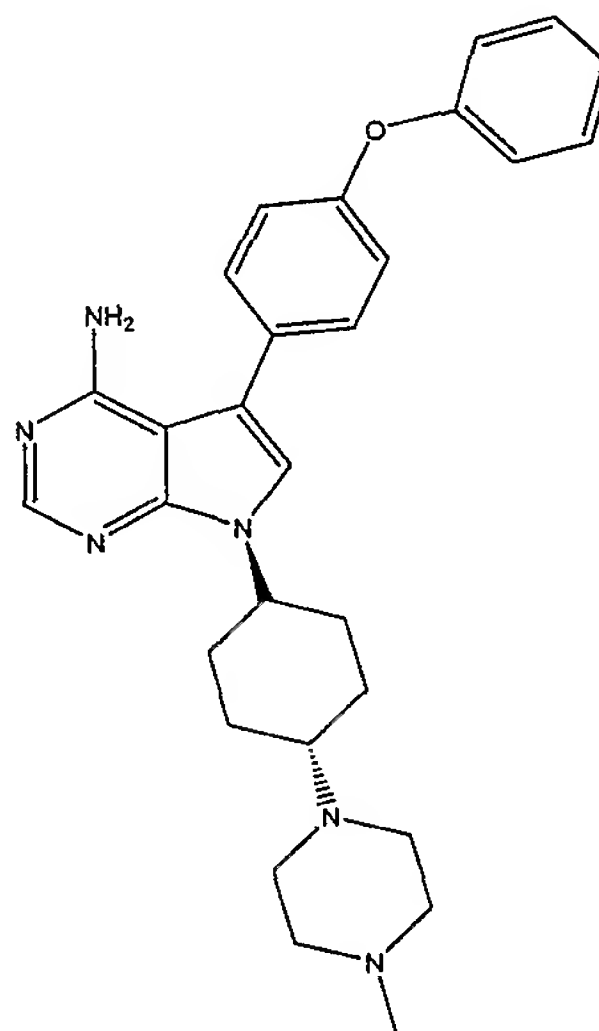
-61-



12. The crystalline polypeptide/ligand complex of Claim 11 having unit cell parameters a and b are about 86.0 Å, and c is about 112.0 Å and $\alpha = \beta = \gamma = 90^\circ$.

5

13. The crystalline polypeptide/ligand complex of Claim 6 wherein the ligand is of the formula:



- 10 14. The crystalline polypeptide/ligand complex of Claim 13 having unit cell parameters a and b are about 86.0 Å, c is about 112.0 Å and $\alpha = \beta = \gamma = 90^\circ$.

15. A method of determining the three dimensional structure of a first polypeptide comprising the catalytic domain of a Tie-2 protein, said method comprising the steps of:
- 5 (a) obtaining a crystal of the first polypeptide comprising the catalytic domain of Tie-2;
- (b) obtaining x-ray diffraction data for said crystal; and
- (c) solving the crystal structure of said crystal using the atomic coordinates of a second polypeptide and said x-ray diffraction data, said second polypeptide comprising the catalytic domain of a Tie-2 protein.
- 10 16. The method of Claim 15 wherein the crystal of the first polypeptide comprises the first polypeptide complexed with a ligand.
- 15 17. The method of Claim 15 wherein the first polypeptide comprises the catalytic domain of a mammalian Tie-2 protein.
18. The method of Claim 17 wherein the first polypeptide and the second polypeptide, independently, comprise the catalytic domain of a human Tie-2 protein.
- 20 19. The method of Claim 18, wherein the first polypeptide comprises the catalytic domain of wild type human Tie-2 and the second polypeptide comprises the catalytic domain of wild type human Tie-2.
- 25 20. The method of Claim 19, wherein the first polypeptide comprises the catalytic domain of wild type human Tie-2.
21. A method of identifying a compound which is an inhibitor of a Tie-2 protein, said method comprising the steps of
- 30 (a) obtaining the atomic coordinates of a crystal of a polypeptide comprising the catalytic domain of a Tie-2 protein;

- (b) using said atomic coordinates to define the active subsites of Tie-2; and
- (c) identifying a compound which binds to the one or more active subsite; wherein the compound which bind to the active subsite or sites is an inhibitor of a Tie-2 protein.

5

22. The method of Claim 21, further comprising the step of

- (d) assessing the ability of the compound identified in step (c) to inhibit Tie-2.

10

23. The method of Claim 21 wherein the Tie-2 protein is a mammalian protein.

24. The method of Claim 22 wherein the Tie-2 protein is a human protein.

25. The method of Claim 24, wherein the Tie-2 protein is wild type human Tie-2.

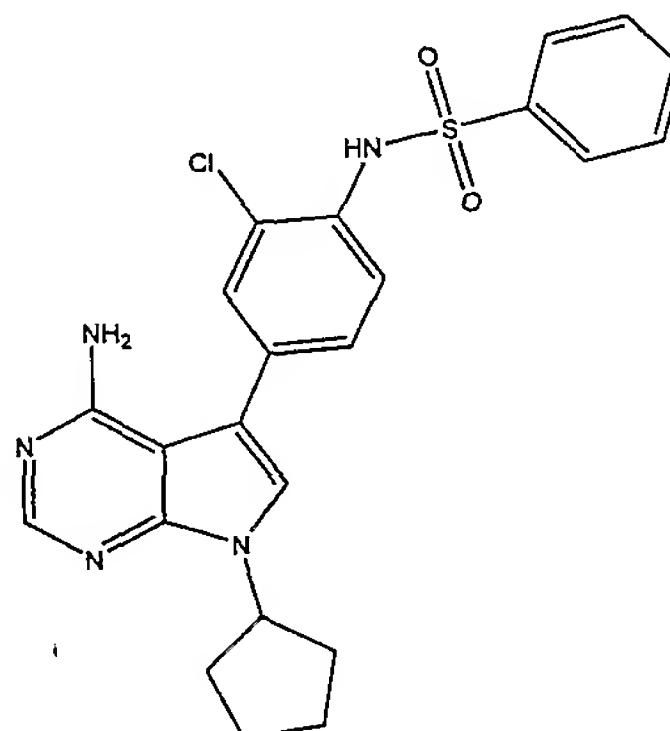
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26. The method of Claim 21 wherein said crystal further comprises a ligand bound to said catalytic domain.

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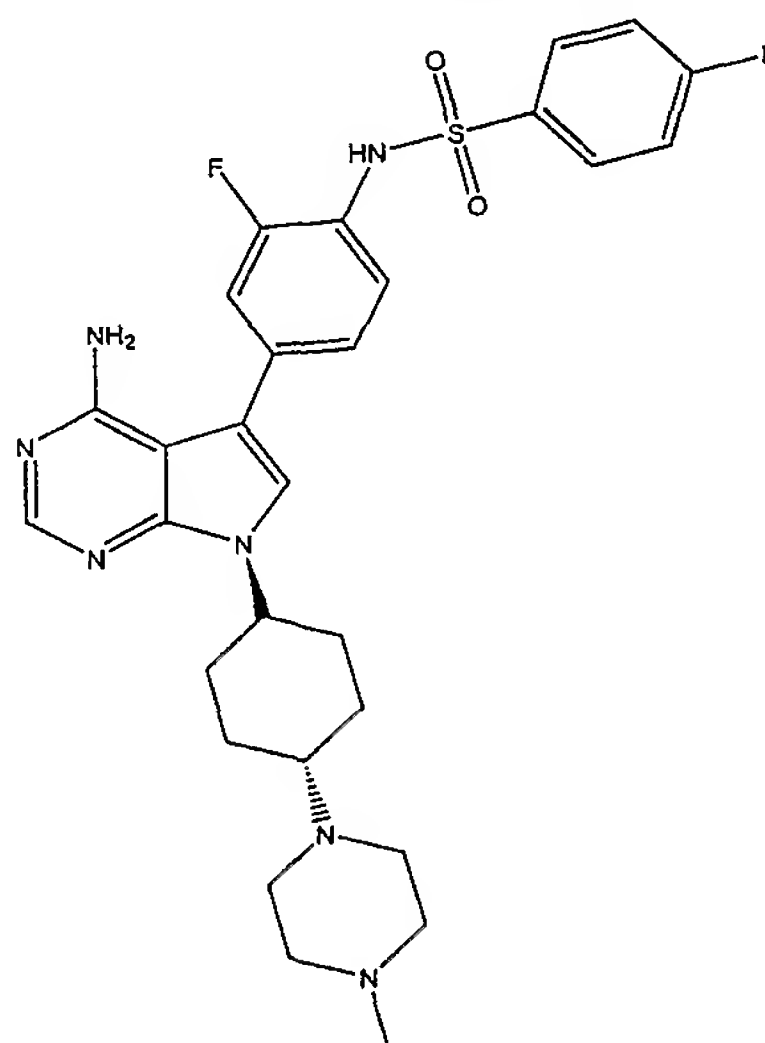
27. The method of Claim 24 wherein the polypeptide comprises amino acids 802-1124 of SEQ ID NO: 1.

28. The method of Claim 24, wherein the ligand is of the formula:



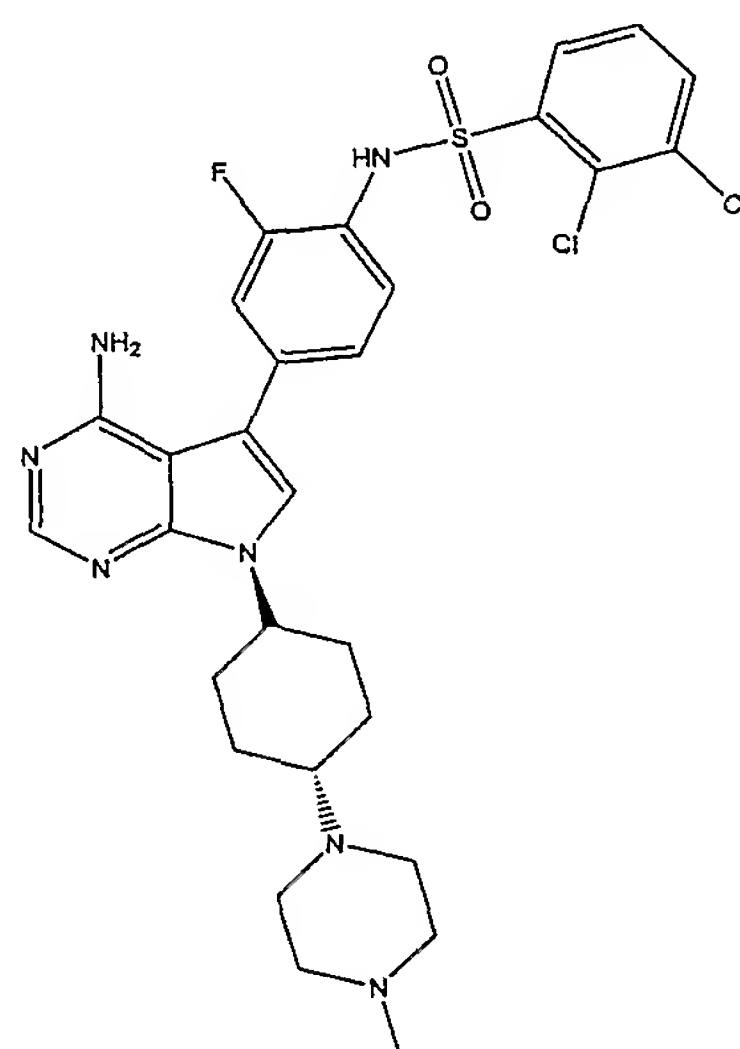
29. The method of Claim 28, wherein the crystal has unit cell parameters wherein a is about 96 Å, b is about 118 Å, c is about 78 Å and $\alpha = \beta = \gamma = 90^\circ$.

5 30. The method of Claim 24, wherein the ligand is of the formula:



31. The method of Claim 30, wherein the crystal has unit cell parameters wherein a and b are about 86.0 Å, c is about 112.0 Å and $\alpha = \beta = \gamma = 90^\circ$.

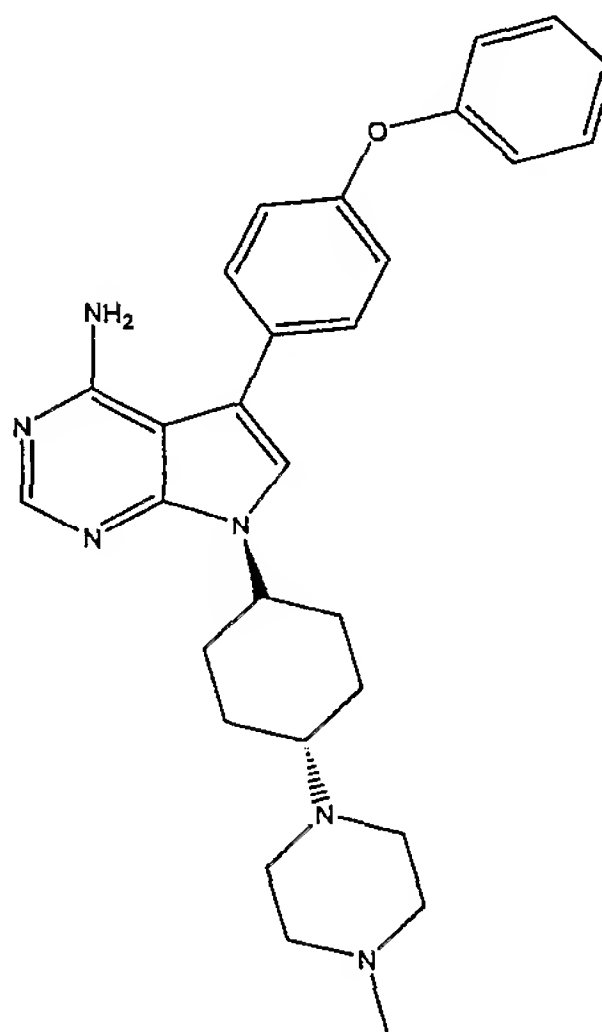
10 32. The method of Claim 24, wherein the ligand is of the formula:



33. The method of Claim 32, wherein the crystal has unit cell parameters wherein

a and b are about 86.0 Å, and c is about 112.0 Å and $\alpha = \beta = \gamma = 90^\circ$.

34. The method of Claim 24, wherein the ligand is of the formula:



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35. The method of Claim 34, wherein the crystal has unit cell parameters wherein a and b are about 86.0 Å, c is about 112.0 Å and $\alpha = \beta = \gamma = 90^\circ$.

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36. A method of identifying a compound which is a potential inhibitor of a Tie-2 protein, said method comprising the step of designing a compound that will interact with one or more subsites in the catalytic domain of the Tie-2 protein, based upon the crystal structure coordinates of a polypeptide comprising the catalytic domain; wherein said compound is identified as a potential inhibitor of the Tie-2 protein.

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37. The method of Claim 36 wherein the Tie-2 protein is a mammalian Tie-2 protein.

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38. The method of Claim 37 wherein the Tie-2 protein is a human Tie-2 protein.
39. The method of Claim 38, wherein the Tie-2 protein is wild type human Tie-2.

40. The method of Claim 39 wherein the polypeptide comprises amino acids 802-1124 of SEQ ID NO: 1.
- 5 41. The method of Claim 38 wherein the crystal structure coordinates are set forth in Fig. 3.
42. The method of Claim 38 wherein the crystal structure coordinates are set forth in Fig. 4.
- 10 43. The method of Claim 38 wherein the crystal structure coordinates are set forth in Fig. 5.
44. The method of Claim 38 wherein the crystal structure coordinates are set forth in Fig. 6.
- 15 45. The method of Claim 38 wherein the compound interacts with one or more of subsites 1 to 9.
- 20 46. The method of Claim 45 wherein the compound interacts with two or more of subsites 1 to 9.
47. The method of Claim 46 wherein the compound interacts with three or more of subsites 1 to 9.
- 25 48. The method of Claim 46 wherein the compound interacts with a set of subsites comprising subsite 1 and subsite 2.
49. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2 and subsite 3.

50. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2 and subsite 8.
- 5 51. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2, subsite 3 and subsite 8.
52. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 4 and subsite 5.
- 10 53. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2, subsite 7 and subsite 8.
54. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2, subsite 3, subsite 7 and subsite 8.
- 15 55. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2, subsite 3, subsite 7 and subsite 8.
- 20 56. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2, subsite 4, subsite 6 and subsite 8.
57. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2, subsite 3, subsite 4, subsite 6 and subsite 8.
- 25 58. The method of Claim 47 wherein the compound interacts with a set of subsites comprising subsite 1, subsite 2, subsite 3, subsite 4, subsite 6 and subsite 8.
59. A Tie-2 inhibitor comprising two or more of the following:
- 30 (a) a hydrogen bond donor positioned to interact with Glu 903 of human Tie-2;

- (b) a hydrogen bond acceptor positioned to interact with Ala 905 of human Tie-2;
- (c) a hydrogen bond donor positioned to interact with Ala 905 of human Tie-2;
- 5 (d) a hydrophobic moiety positioned to interact with one or more of Ile 830, Val 838, Ala 853, Ile 886, Ile 902, Tyr 904, Ala 905 and Leu 971 of human Tie-2;
- (e) a hydrogen bond donor or positively charged functional group positioned to interact with Asp 912 of human Tie-2;
- 10 (f) a hydrogen bond donor or hydrogen bond acceptor positioned to interact with Asn 909 of human Tie-2;
- (g) a hydrophobic moiety positioned to interact with one or more of Val 838, Lys 855, Ile 886, Ile 902, Leu 971 and Ala 981 of human Tie-2;
- (h) a hydrogen bond acceptor or negatively charged functional group positioned to interact with Lys 855 of human Tie-2;
- 15 (i) a hydrogen bond acceptor positioned to interact with Asp 982 of human Tie-2;
- (j) a hydrogen bond acceptor positioned to interact with Phe 983 of human Tie-2;
- 20 (k) a hydrophobic moiety positioned to interact with one or more of Leu 873, Leu 876, Ile 885, Ile 886, Leu 888, Leu 900, Ile 902, Ala 981 and Phe 983 of human Tie-2;
- (l) a hydrogen bond donor or positively charged functional group positioned to interact with Asp 982 of human Tie-2;
- 25 (m) a hydrogen bond donor positioned to interact with Ile 886 of human Tie-2;
- (n) a hydrogen bond donor positioned to interact with Leu 768 of human Tie-2;
- (o) a hydrogen bond acceptor positioned to interact with Gly 831 of human Tie-2;
- 30 (p) a hydrogen bond donor or positively charged functional group

positioned to interact with Glu 832 of human Tie-2;

(q) a hydrogen bond acceptor or negatively charged functional group positioned to interact with Lys 840 of human Tie-2;

(r) a hydrogen bond acceptor or negatively charged functional group positioned to interact with Lys 916 of human Tie-2;

(s) a hydrogen bond acceptor or negatively charged functional group positioned to interact with Arg 968 of human Tie-2;

(t) a hydrogen bond donor positioned to interact with Arg 968 of human Tie-2.

10

60. The Tie-2 inhibitor of Claim 59 comprising (b) and (d).

61. The Tie-2 inhibitor of Claim 59 comprising (d) and at least one of (a), (b) and (c).

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62. The Tie-2 inhibitor of Claim 59 comprising (d) and at least two of (a), (b) and (c).

63. The Tie-2 inhibitor of Claim 62 further comprising at least one of (e) and (f).

20

64. The Tie-2 inhibitor of Claim 62 further comprising (g).

65. The Tie-2 inhibitor of Claim 63 further comprising (g).

25

66. The Tie-2 inhibitor of Claim 64 further comprising (k).

67. The Tie-2 inhibitor of Claim 65 further comprising (k).

68. The Tie-2 inhibitor of Claim 62 further comprising at least one of (i) and (j).

30

69. The Tie-2 inhibitor of Claim 63 further comprising at least one of (i) and (j).

70. The Tie-2 inhibitor of Claim 66 further comprising at least one of (i) and (j).
71. The Tie-2 inhibitor of Claim 67 further comprising at least one of (i) and (j).
- 5 72. The Tie-2 inhibitor of Claim 59, wherein the inhibitor has a K_i of at least about 1 mM.
73. The Tie-2 inhibitor of Claim 59, wherein the inhibitor has a K_i of at least about 100 μ M.
- 10 74. The Tie-2 inhibitor of Claim 59, wherein the inhibitor has a K_i of at least about 10 μ M.
- 15 75. The Tie-2 inhibitor of Claim 59, wherein the inhibitor selectively binds Tie-2 receptors.
76. A method of treating a Tie-2 dependent condition in a patient comprising the step of administering to the patient a therapeutically effective amount of a Tie-2 inhibitor of Claim 59.
- 20 77. The method of Claim 76 wherein the patient is a human.
78. The method of Claim 76 wherein the Tie-2 dependent condition is characterized by excessive vascular proliferation.
- 25 79. The method of Claim 78 wherein the Tie-2 dependent condition is a hyperproliferative disorder, cancer, a cardiovascular condition, an ocular condition, von Hippel Lindau disease, pemphigoid, psoriasis, Paget's disease, polycystic kidney disease, fibrosis, sarcoidosis, cirrhosis, thyroiditis, Osler-Weber-Rendu disease, chronic inflammation, synovitis, inflammatory bowel disease, Crohn's disease, rheumatoid arthritis, osteoarthritis, psoriatic arthritis,
- 30

an ulcer or sepsis.

- 80 . The method of Claim 79, wherein the condition is a cancer selected from the group consisting of solid tumor, a sarcoma, fibrosarcoma, osteoma, melanoma, retinoblastoma, a rhabdomyosarcoma, glioblastoma, neuroblastoma, teratocarcinoma, an hematopoietic malignancy, malignant ascites, Kaposi's sarcoma, Hodgkin's disease, lymphoma, myeloma and leukemia.
- 5
- 81 . The method of Claim 79 wherein the condition is a cardiovascular condition selected from the group consisting of atherosclerosis, restenosis, ischemia/reperfusion injury, chronic occlusive pulmonary disease, vascular occlusion, carotid obstructive disease, Crow-Fukase (POEMS) syndrome, anemia, ischemia, infarct, and vascular leakage disorders.
- 10
- 82 . The method of Claim 79 wherein the condition is an ocular condition selected from the group consisting of ocular or macular edema, ocular neovascular disease, scleritis, radial keratotomy, uveitis, vitritis, myopia, optic pits, chronic retinal detachment, post-laser treatment complications, conjunctivitis, Stargardt's disease, Eales disease, retinopathy, macular degeneration and microangiopathy.
- 15
- 20
- 83 . The method of Claim 76, wherein the disorder involves aberrant endothelial-peri-endothelial interactions.
- 25
- 84 . A method of decreasing fertility in a patient comprising the step of administering to the patient a therapeutically effective amount of a Tie-2 inhibitor of Claim 59.

85. A method of promoting angiogenesis or vasculogenesis in a patient comprising the step of administering to the patient a therapeutically effective amount of a Tie-2 inhibitor of Claim 59.
- 5
86. The method of Claim 85, wherein the Tie-2 inhibitor is administered in combination with a pro-angiogenic growth factor.
87. A method of determining the three dimensional structure of a polypeptide comprising the catalytic domain of a Tie-2 protein, said method comprising the steps of:
- 10
- (a) obtaining a crystal of the polypeptide comprising the catalytic domain of Tie-2;
 - (b) obtaining x-ray diffraction data for said crystal; and
 - 15 (c) solving the crystal structure of said crystal.
88. A crystalline polypeptide, said polypeptide comprising a sequence having 80% homology with the catalytic domain of a Tie-2 protein.

.MDSLASLVLC GVSLLLSGTV EGAMDLILIN SLPLVSDAET SLTCIASGWR PHEPITIGRD
FEALMNQHQD PLEVTDQDVTR EWAKKVVWKR EKASKINGAY FCEGRVVRGEA IRIRTMKMRQ
QASFLPATLT MTVDKGDNVN ISFKKVLKE EDAVIYKNGS FIHSVPRHEV PDILEVHLPH
AQPQDAGVYS ARYIGGNLFT SAFTRLIVRR CEAQKWGPEC NHLCTACMNN GVCHEDTGEC
ICPPGFMGRT CEKACELHTF GRTCKERCSG QEGCKSYVFC LPDPYGCSCA TGWKGLQCNE
ACHPGFYGPD CKLRCSCNNG EMCDRFQGCL CSPGWQGLQC EREGIPRMTP KIVDLDPDHIE
VNSGKFNPIC KASGWPLPTN EEMTLVKPDG TVLHPKDFNH TDHFSVAIFT IHRILPPDSG
VWVCSVNTVA GMVEKPFNIS VKVLPKPLNA PNVIDTGHNF AVINISSEPY FGDGPIKSKK
LLYKPVNHYE AWQHIQVTNE IVTLNYLEPR TEYELCVQLV RRGEKGEGHP GPVRRFTTAS
IGLPPPRGLN LLPKSQTTLN LTWQPIFPSS EDDFYVEVER RSVQKSDQQN IKVPGNLTSV
LLNNLHPREQ YVVRARVNTK AQGEWSEDLT AWTLSDILPP QPENIKISNI THSSAVISWT
ILDGYSISSI TIRYKVQGKN EDQHVDVKIK NATIIQYQLK GLEPETAYQV DIFAENNIGS
SNPAFSHELV TLPESQAPAD LGGKMLLIA ILGSAGMTCL TVLLAFLIIL QLKRANVQRR
MAQAFQNVRE EPAVQFNSGT LALNRKVKN PDPTIYPVLD WNDIKFQDVI GEGNFCQVLK
ARIKKDGLRM DAAIKRMKEY ASKDDHRDFA GELEVLCKLG HHPNIINLLG ACEHRGYLYL
AIEYAPHGNL LDFLRKSRVL ETDPAFAIAN STASTLSSQQ LLHFAADVAR GMDYLSQKQF
IHRDLAARNI LVGENYVAKI ADFGLSRGQE VYVKKTMGRL PVRWMAIESL NYSVYTTNSD
VWSYGVLLWE IVSLGGTPYC GMTCAELYEK LPQGYRLEKP LNCDDDEVYDL MRQCWREKPY
ERPSFAQILV SLNRMLEERK TYVNTTLYEK FTYAGIDCSA EEAA

FIG. 1

ALNRKVKNN	PDPTIYPVLD	WNDIKFQDVI	GEGNFGQVLK
ARIKKDGLRM	DAAIKRMKEY	ASKDDHRDFA	GELEVLCKLG
HHPNIINLLG	ACEHRGYLYL	AIEYAPHGNL	LDFLRKSRVL
ETDPAFAIAN	STASTLSSQQ	LLHFAADVAR	GMDYLSQKQF
IHRNLAARNI	LVGENYVAKI	ADFGLSRGQE	VYVKKTMGRL
PVRWMAIESL	NYSVYTTNSD	VWSYGVLLWE	IVSLGGTPYC
GMTCAELYEK	LPQGYRLEKP	LNCDDDEVYDL	MRQCWREKPY
ERPSFAQILV	SLNRMLEERK	TYVNTTLYEK	FTYAGIDCSA
EEAA			

FIG. 2

CRYST1	95.604	117.589	78.214	90.00	90.00	90.00			
ORIGX1	1.000000	0.000000	0.000000			0.000000			
ORIGX2	0.000000	1.000000	0.000000			0.000000			
ORIGX3	0.000000	0.000000	1.000000			0.000000			
SCALE1	0.010460	0.000000	0.000000			0.000000			
SCALE2	0.000000	0.008504	0.000000			0.000000			
SCALE3	0.000000	0.000000	0.012785			0.000000			
ATOM	1	CB	VAL	818	5.159	51.390	-17.822	1.00	65.41 6
ATOM	2	C	VAL	818	3.553	51.091	-15.926	1.00	99.70 6
ATOM	3	O	VAL	818	2.603	51.682	-16.444	1.00	99.70 8
ATOM	4	N	VAL	818	4.074	49.203	-17.428	1.00	99.70 7
ATOM	5	CA	VAL	818	4.628	50.419	-16.774	1.00	99.70 6
ATOM	6	N	LEU	819	3.729	50.991	-14.616	1.00	100.00 7
ATOM	7	CA	LEU	819	2.912	51.555	-13.639	1.00	100.00 6
ATOM	8	CB	LEU	819	3.310	51.175	-12.250	1.00	77.77 6
ATOM	9	CG	LEU	819	2.625	51.796	-11.045	1.00	67.90 6
ATOM	10	CD1	LEU	819	1.161	51.416	-11.022	1.00	67.90 6
ATOM	11	CD2	LEU	819	3.336	51.313	-9.810	1.00	67.90 6
ATOM	12	C	LEU	819	2.607	53.076	-13.729	1.00	100.00 6
ATOM	13	O	LEU	819	3.568	53.838	-13.899	1.00	100.00 8
ATOM	14	N	ASP	820	1.351	53.507	-13.602	1.00	100.00 7
ATOM	15	CA	ASP	820	0.990	54.928	-13.659	1.00	100.00 6
ATOM	16	CB	ASP	820	-0.505	55.084	-13.929	1.00	100.00 6
ATOM	17	CG	ASP	820	-0.910	56.525	-14.140	1.00	100.00 6
ATOM	18	OD1	ASP	820	-2.054	56.874	-13.785	1.00	100.00 8
ATOM	19	OD2	ASP	820	-0.087	57.303	-14.663	1.00	100.00 8
ATOM	20	C	ASP	820	1.314	55.593	-12.329	1.00	100.00 6
ATOM	21	O	ASP	820	0.786	55.200	-11.290	1.00	100.00 8
ATOM	22	N	TRP	821	2.171	56.605	-12.361	1.00	100.00 7
ATOM	23	CA	TRP	821	2.558	57.278	-11.132	1.00	100.00 6
ATOM	24	CB	TRP	821	3.291	58.582	-11.458	1.00	96.30 6
ATOM	25	CG	TRP	821	3.985	59.118	-10.263	1.00	96.04 6
ATOM	26	CD2	TRP	821	3.369	59.782	-9.149	1.00	96.04 6
ATOM	27	CE2	TRP	821	4.371	59.991	-8.185	1.00	96.04 6
ATOM	28	CE3	TRP	821	2.061	60.200	-8.869	1.00	96.04 6
ATOM	29	CD1	TRP	821	5.302	58.974	-9.938	1.00	96.04 6
ATOM	30	NE1	TRP	821	5.545	59.494	-8.689	1.00	96.04 7
ATOM	31	CZ2	TRP	821	4.106	60.614	-6.976	1.00	96.04 6
ATOM	32	CZ3	TRP	821	1.803	60.816	-7.657	1.00	96.04 6
ATOM	33	CH2	TRP	821	2.824	61.007	-6.733	1.00	96.04 6
ATOM	34	C	TRP	821	1.355	57.543	-10.207	1.00	100.00 6
ATOM	35	O	TRP	821	1.462	57.434	-8.983	1.00	100.00 8
ATOM	36	N	ASN	822	0.207	57.853	-10.801	1.00	78.55 7
ATOM	37	CA	ASN	822	-1.018	58.149	-10.061	1.00	78.55 6
ATOM	38	CB	ASN	822	-2.158	58.380	-11.037	1.00	100.00 6
ATOM	39	CG	ASN	822	-3.126	59.416	-10.546	1.00	100.00 6
ATOM	40	OD1	ASN	822	-3.508	60.321	-11.291	1.00	100.00 8
ATOM	41	ND2	ASN	822	-3.536	59.303	-9.286	1.00	100.00 7
ATOM	42	C	ASN	822	-1.453	57.094	-9.048	1.00	78.55 6
ATOM	43	O	ASN	822	-1.451	57.340	-7.842	1.00	78.55 8
ATOM	44	N	ASP	823	-1.854	55.933	-9.554	1.00	95.03 7
ATOM	45	CA	ASP	823	-2.308	54.841	-8.704	1.00	95.03 6
ATOM	46	CB	ASP	823	-2.991	53.775	-9.562	1.00	65.89 6
ATOM	47	C	ASP	823	-1.158	54.218	-7.916	1.00	95.03 6

FIG. 3A

ATOM	48	O	ASP	823	-0.967	53.008	-7.949	1.00	95.03	8
ATOM	49	N	ILE	824	-0.384	55.043	-7.221	1.00	88.67	7
ATOM	50	CA	ILE	824	0.729	54.531	-6.426	1.00	88.67	6
ATOM	51	CB	ILE	824	2.112	54.819	-7.082	1.00	53.67	6
ATOM	52	CG2	ILE	824	3.202	54.080	-6.326	1.00	56.64	6
ATOM	53	CG1	ILE	824	2.161	54.314	-8.526	1.00	56.64	6
ATOM	54	CD1	ILE	824	3.503	54.615	-9.196	1.00	56.64	6
ATOM	55	C	ILE	824	0.701	55.176	-5.041	1.00	88.67	6
ATOM	56	O	ILE	824	1.617	55.912	-4.665	1.00	88.67	8
ATOM	57	N	LYS	825	-0.361	54.889	-4.292	1.00	65.97	7
ATOM	58	CA	LYS	825	-0.552	55.426	-2.947	1.00	65.97	6
ATOM	59	CB	LYS	825	-1.917	54.995	-2.406	1.00	30.30	6
ATOM	60	C	LYS	825	0.544	55.003	-1.973	1.00	65.97	6
ATOM	61	O	LYS	825	0.502	53.909	-1.401	1.00	65.97	8
ATOM	62	N	PHE	826	1.526	55.879	-1.788	1.00	96.52	7
ATOM	63	CA	PHE	826	2.632	55.608	-0.878	1.00	96.52	6
ATOM	64	CB	PHE	826	3.784	56.586	-1.112	1.00	96.59	6
ATOM	65	CG	PHE	826	4.397	56.474	-2.463	1.00	100.00	6
ATOM	66	CD1	PHE	826	3.989	57.310	-3.489	1.00	100.00	6
ATOM	67	CD2	PHE	826	5.351	55.500	-2.726	1.00	100.00	6
ATOM	68	CE1	PHE	826	4.518	57.181	-4.764	1.00	100.00	6
ATOM	69	CE2	PHE	826	5.888	55.358	-4.001	1.00	100.00	6
ATOM	70	CZ	PHE	826	5.469	56.202	-5.023	1.00	100.00	6
ATOM	71	C	PHE	826	2.158	55.727	0.565	1.00	96.52	6
ATOM	72	O	PHE	826	1.746	56.794	0.991	1.00	96.52	8
ATOM	73	N	GLN	827	2.247	54.651	1.332	1.00	100.00	7
ATOM	74	CA	GLN	827	1.769	54.708	2.698	1.00	100.00	6
ATOM	75	CB	GLN	827	0.886	53.484	2.937	1.00	100.00	6
ATOM	76	CG	GLN	827	-0.252	53.407	1.903	1.00	100.00	6
ATOM	77	CD	GLN	827	-1.539	52.860	2.488	1.00	100.00	6
ATOM	78	OE1	GLN	827	-1.553	51.771	3.060	1.00	100.00	8
ATOM	79	NE2	GLN	827	-2.633	53.615	2.349	1.00	100.00	7
ATOM	80	C	GLN	827	2.840	54.886	3.781	1.00	100.00	6
ATOM	81	O	GLN	827	2.892	55.942	4.395	1.00	100.00	8
ATOM	82	N	ASP	828	3.696	53.894	4.015	1.00	99.72	7
ATOM	83	CA	ASP	828	4.713	54.034	5.064	1.00	99.72	6
ATOM	84	CB	ASP	828	4.144	53.510	6.388	1.00	87.03	6
ATOM	85	CG	ASP	828	5.121	53.627	7.533	1.00	84.60	6
ATOM	86	OD1	ASP	828	5.870	54.617	7.572	1.00	84.60	8
ATOM	87	OD2	ASP	828	5.128	52.740	8.406	1.00	84.60	8
ATOM	88	C	ASP	828	6.003	53.286	4.720	1.00	99.72	6
ATOM	89	O	ASP	828	5.961	52.262	4.034	1.00	99.72	8
ATOM	90	N	VAL	829	7.154	53.772	5.178	1.00	85.45	7
ATOM	91	CA	VAL	829	8.408	53.075	4.863	1.00	85.45	6
ATOM	92	CB	VAL	829	9.606	53.874	5.391	1.00	51.35	6
ATOM	93	C	VAL	829	8.460	51.633	5.402	1.00	85.45	6
ATOM	94	O	VAL	829	8.437	51.418	6.615	1.00	85.45	8
ATOM	95	N	ILE	830	8.538	50.663	4.488	1.00	100.00	7
ATOM	96	CA	ILE	830	8.598	49.244	4.852	1.00	100.00	6
ATOM	97	CB	ILE	830	8.745	48.326	3.602	1.00	100.00	6
ATOM	98	CG2	ILE	830	9.458	47.031	3.973	1.00	81.07	6
ATOM	99	CG1	ILE	830	7.370	48.034	2.994	1.00	81.07	6
ATOM	100	CD1	ILE	830	6.385	47.414	3.969	1.00	81.07	6
ATOM	101	C	ILE	830	9.788	49.013	5.769	1.00	100.00	6
ATOM	102	O	ILE	830	9.782	48.103	6.596	1.00	100.00	8
ATOM	103	N	GLY	831	10.821	49.834	5.605	1.00	95.79	7
ATOM	104	CA	GLY	831	11.992	49.713	6.453	1.00	95.79	6

FIG. 3B

ATOM	105	C	GLY	831	13.352	49.743	5.806	1.00	95.79	6
ATOM	106	O	GLY	831	13.497	50.005	4.613	1.00	95.79	8
ATOM	107	N	GLU	832	14.357	49.480	6.630	1.00	99.78	7
ATOM	108	CA	GLU	832	15.760	49.427	6.231	1.00	99.78	6
ATOM	109	CB	GLU	832	16.055	48.055	5.602	1.00	100.00	6
ATOM	110	CG	GLU	832	16.417	46.997	6.632	1.00	100.00	6
ATOM	111	CD	GLU	832	17.103	47.598	7.859	1.00	100.00	6
ATOM	112	OE1	GLU	832	16.380	48.153	8.721	1.00	100.00	8
ATOM	113	OE2	GLU	832	18.352	47.535	7.943	1.00	100.00	8
ATOM	114	C	GLU	832	16.376	50.502	5.339	1.00	99.78	6
ATOM	115	O	GLU	832	15.689	51.284	4.679	1.00	99.78	8
ATOM	116	N	GLY	833	17.708	50.501	5.333	1.00	100.00	7
ATOM	117	CA	GLY	833	18.494	51.424	4.536	1.00	100.00	6
ATOM	118	C	GLY	833	19.580	50.682	3.756	1.00	100.00	6
ATOM	119	O	GLY	833	19.557	49.446	3.693	1.00	100.00	8
ATOM	120	N	ASN	834	20.540	51.432	3.192	1.00	100.00	7
ATOM	121	CA	ASN	834	21.643	50.854	2.407	1.00	100.00	6
ATOM	122	CB	ASN	834	22.414	49.810	3.241	1.00	100.00	6
ATOM	123	CG	ASN	834	23.700	49.360	2.579	1.00	100.00	6
ATOM	124	OD1	ASN	834	23.727	49.066	1.387	1.00	100.00	8
ATOM	125	ND2	ASN	834	24.778	49.302	3.354	1.00	100.00	7
ATOM	126	C	ASN	834	21.094	50.179	1.149	1.00	100.00	6
ATOM	127	O	ASN	834	20.299	49.228	1.240	1.00	100.00	8
ATOM	128	N	PHE	835	21.519	50.650	-0.030	1.00	100.00	7
ATOM	129	CA	PHE	835	21.056	50.117	-1.328	1.00	100.00	6
ATOM	130	CB	PHE	835	22.041	49.061	-1.877	1.00	100.00	6
ATOM	131	CG	PHE	835	23.383	49.629	-2.294	1.00	100.00	6
ATOM	132	CD1	PHE	835	24.562	48.976	-1.954	1.00	100.00	6
ATOM	133	CD2	PHE	835	23.465	50.835	-2.996	1.00	100.00	6
ATOM	134	CE1	PHE	835	25.808	49.509	-2.291	1.00	100.00	6
ATOM	135	CE2	PHE	835	24.706	51.380	-3.342	1.00	100.00	6
ATOM	136	CZ	PHE	835	25.879	50.718	-2.987	1.00	100.00	6
ATOM	137	C	PHE	835	19.641	49.519	-1.261	1.00	100.00	6
ATOM	138	O	PHE	835	19.380	48.467	-1.841	1.00	100.00	8
ATOM	139	N	GLY	836	18.748	50.228	-0.570	1.00	100.00	7
ATOM	140	CA	GLY	836	17.369	49.813	-0.397	1.00	100.00	6
ATOM	141	C	GLY	836	16.689	50.596	0.720	1.00	100.00	6
ATOM	142	O	GLY	836	17.188	50.622	1.840	1.00	100.00	8
ATOM	143	N	GLN	837	15.571	51.261	0.418	1.00	100.00	7
ATOM	144	CA	GLN	837	14.831	52.043	1.420	1.00	100.00	6
ATOM	145	CB	GLN	837	15.333	53.505	1.397	1.00	100.00	6
ATOM	146	CG	GLN	837	14.344	54.609	1.081	1.00	100.00	6
ATOM	147	CD	GLN	837	15.041	55.948	0.852	1.00	100.00	6
ATOM	148	OE1	GLN	837	15.798	56.108	-0.108	1.00	100.00	8
ATOM	149	NE2	GLN	837	14.796	56.912	1.739	1.00	100.00	7
ATOM	150	C	GLN	837	13.327	51.889	1.138	1.00	100.00	6
ATOM	151	O	GLN	837	12.525	52.818	1.236	1.00	100.00	8
ATOM	152	N	VAL	838	12.993	50.652	0.789	1.00	49.78	7
ATOM	153	CA	VAL	838	11.645	50.199	0.469	1.00	49.78	6
ATOM	154	CB	VAL	838	11.565	48.683	0.604	1.00	54.51	6
ATOM	155	CG1	VAL	838	11.159	48.064	-0.703	1.00	54.51	6
ATOM	156	CG2	VAL	838	12.902	48.146	1.071	1.00	54.51	6
ATOM	157	C	VAL	838	10.515	50.785	1.303	1.00	49.78	6
ATOM	158	O	VAL	838	10.694	51.096	2.481	1.00	49.78	8
ATOM	159	N	LEU	839	9.344	50.916	0.684	1.00	44.19	7
ATOM	160	CA	LEU	839	8.171	51.461	1.369	1.00	44.19	6
ATOM	161	CB	LEU	839	7.935	52.921	0.962	1.00	90.21	6

FIG. 3C

ATOM	162	CG	LEU	839	9.039	53.975	1.060	1.00	84.90	6
ATOM	163	CD1	LEU	839	10.061	53.788	-0.028	1.00	84.90	6
ATOM	164	CD2	LEU	839	8.417	55.343	0.924	1.00	84.90	6
ATOM	165	C	LEU	839	6.900	50.671	1.061	1.00	44.19	6
ATOM	166	O	LEU	839	6.814	50.010	0.033	1.00	44.19	8
ATOM	167	N	LYS	840	5.920	50.740	1.959	1.00	64.49	7
ATOM	168	CA	LYS	840	4.642	50.068	1.744	1.00	64.49	6
ATOM	169	CB	LYS	840	3.953	49.727	3.066	1.00	84.80	6
ATOM	170	CG	LYS	840	2.531	49.222	2.900	1.00	81.21	6
ATOM	171	CD	LYS	840	2.073	48.506	4.142	1.00	81.21	6
ATOM	172	CE	LYS	840	0.582	48.660	4.331	1.00	81.21	6
ATOM	173	NZ	LYS	840	-0.153	48.279	3.096	1.00	81.21	7
ATOM	174	C	LYS	840	3.798	51.053	0.951	1.00	64.49	6
ATOM	175	O	LYS	840	3.854	52.260	1.176	1.00	64.49	8
ATOM	176	N	ALA	841	3.021	50.538	0.016	1.00	53.58	7
ATOM	177	CA	ALA	841	2.219	51.409	-0.814	1.00	53.58	6
ATOM	178	CB	ALA	841	3.082	51.913	-1.961	1.00	25.05	6
ATOM	179	C	ALA	841	1.003	50.670	-1.353	1.00	53.58	6
ATOM	180	O	ALA	841	1.144	49.616	-1.966	1.00	53.58	8
ATOM	181	N	ARG	842	-0.189	51.212	-1.135	1.00	86.10	7
ATOM	182	CA	ARG	842	-1.385	50.551	-1.637	1.00	86.10	6
ATOM	183	CB	ARG	842	-2.630	51.062	-0.905	1.00	40.66	6
ATOM	184	C	ARG	842	-1.514	50.804	-3.137	1.00	86.10	6
ATOM	185	O	ARG	842	-2.277	51.662	-3.572	1.00	86.10	8
ATOM	186	N	ILE	843	-0.763	50.040	-3.918	1.00	81.66	7
ATOM	187	CA	ILE	843	-0.773	50.176	-5.372	1.00	81.66	6
ATOM	188	CB	ILE	843	0.612	49.831	-5.984	1.00	100.00	6
ATOM	189	CG2	ILE	843	0.443	49.166	-7.362	1.00	100.00	6
ATOM	190	CG1	ILE	843	1.469	51.092	-6.056	1.00	100.00	6
ATOM	191	CD1	ILE	843	1.562	51.810	-4.732	1.00	100.00	6
ATOM	192	C	ILE	843	-1.796	49.337	-6.116	1.00	81.66	6
ATOM	193	O	ILE	843	-1.940	48.137	-5.884	1.00	81.66	8
ATOM	194	N	LYS	844	-2.482	49.988	-7.041	1.00	89.28	7
ATOM	195	CA	LYS	844	-3.449	49.324	-7.893	1.00	89.28	6
ATOM	196	CB	LYS	844	-4.657	50.218	-8.114	1.00	80.56	6
ATOM	197	C	LYS	844	-2.695	49.129	-9.205	1.00	89.28	6
ATOM	198	O	LYS	844	-1.818	49.928	-9.538	1.00	89.28	8
ATOM	199	N	LYS	845	-3.022	48.079	-9.944	1.00	100.00	7
ATOM	200	CA	LYS	845	-2.339	47.828	-11.208	1.00	100.00	6
ATOM	201	CB	LYS	845	-1.937	46.355	-11.305	1.00	100.00	6
ATOM	202	C	LYS	845	-3.232	48.203	-12.376	1.00	100.00	6
ATOM	203	O	LYS	845	-3.957	49.206	-12.324	1.00	100.00	8
ATOM	204	N	ASP	846	-2.834	47.343	-13.559	1.00	100.00	7
ATOM	205	CA	ASP	846	-3.726	47.631	-14.691	1.00	100.00	6
ATOM	206	CB	ASP	846	-3.314	46.796	-15.906	1.00	100.00	6
ATOM	207	CG	ASP	846	-3.993	47.249	-17.201	1.00	100.00	6
ATOM	208	OD1	ASP	846	-4.145	48.507	-17.444	1.00	100.00	8
ATOM	209	OD2	ASP	846	-4.414	46.373	-18.049	1.00	100.00	8
ATOM	210	C	ASP	846	-5.170	47.288	-14.320	1.00	100.00	6
ATOM	211	O	ASP	846	-5.989	46.948	-15.186	1.00	100.00	8
ATOM	212	N	GLY	847	-5.433	47.392	-13.030	1.00	100.00	7
ATOM	213	CA	GLY	847	-6.758	47.112	-12.459	1.00	100.00	6
ATOM	214	C	GLY	847	-6.612	46.491	-11.067	1.00	100.00	6
ATOM	215	O	GLY	847	-5.794	45.583	-10.856	1.00	100.00	8
ATOM	216	N	LEU	848	-7.419	47.011	-10.161	1.00	86.45	7
ATOM	217	CA	LEU	848	-7.450	46.563	-8.761	1.00	86.45	6
ATOM	218	CB	LEU	848	-7.206	45.055	-8.687	1.00	99.14	6

FIG. 3D

ATOM	219	CG	LEU	848	-6.201	44.560	-9.729	1.00	92.74	6
ATOM	220	CD1	LEU	848	-5.757	43.115	-9.491	1.00	92.74	6
ATOM	221	CD2	LEU	848	-6.753	44.595	-11.155	1.00	92.74	6
ATOM	222	C	LEU	848	-6.366	47.280	-7.954	1.00	86.45	6
ATOM	223	O	LEU	848	-5.717	48.215	-8.445	1.00	86.45	8
ATOM	224	N	ARG	849	-6.211	46.809	-6.730	1.00	99.60	7
ATOM	225	CA	ARG	849	-5.226	47.347	-5.780	1.00	99.60	6
ATOM	226	CB	ARG	849	-5.877	48.415	-4.899	1.00	100.00	6
ATOM	227	CG	ARG	849	-6.736	49.403	-5.692	1.00	99.93	6
ATOM	228	CD	ARG	849	-8.059	49.736	-4.998	1.00	99.93	6
ATOM	229	NE	ARG	849	-7.887	50.134	-3.594	1.00	99.93	7
ATOM	230	CZ	ARG	849	-8.903	50.347	-2.746	1.00	99.93	6
ATOM	231	NH1	ARG	849	-10.175	50.205	-3.143	1.00	99.93	7
ATOM	232	NH2	ARG	849	-8.747	50.710	-1.465	1.00	99.93	7
ATOM	233	C	ARG	849	-4.694	46.224	-4.887	1.00	99.60	6
ATOM	234	O	ARG	849	-5.398	45.242	-4.608	1.00	99.60	8
ATOM	235	N	MET	850	-3.457	46.411	-4.467	1.00	80.73	7
ATOM	236	CA	MET	850	-2.754	45.456	-3.599	1.00	80.73	6
ATOM	237	CB	MET	850	-1.967	44.457	-4.450	1.00	100.00	6
ATOM	238	CG	MET	850	-2.734	43.994	-5.690	1.00	68.64	6
ATOM	239	SD	MET	850	-1.849	44.290	-7.206	1.00	68.64	16
ATOM	240	CE	MET	850	-0.189	43.661	-7.074	1.00	68.64	6
ATOM	241	C	MET	850	-1.782	46.199	-2.681	1.00	80.73	6
ATOM	242	O	MET	850	-1.937	47.403	-2.426	1.00	80.73	8
ATOM	243	N	ASP	851	-1.168	45.352	-2.147	1.00	74.44	7
ATOM	244	CA	ASP	851	-0.137	45.775	-1.223	1.00	74.44	6
ATOM	245	CB	ASP	851	-0.163	44.913	0.034	1.00	100.00	6
ATOM	246	CG	ASP	851	-0.724	45.642	1.229	1.00	100.00	6
ATOM	247	OD1	ASP	851	-1.307	46.731	1.026	1.00	100.00	8
ATOM	248	OD2	ASP	851	-0.588	45.124	2.360	1.00	100.00	8
ATOM	249	C	ASP	851	1.159	45.518	-1.967	1.00	74.44	6
ATOM	250	O	ASP	851	1.583	44.367	-2.118	1.00	74.44	8
ATOM	251	N	ALA	852	1.775	46.581	-2.456	1.00	26.66	7
ATOM	252	CA	ALA	852	3.023	46.431	-3.173	1.00	26.66	6
ATOM	253	CB	ALA	852	2.984	47.212	-4.475	1.00	11.17	6
ATOM	254	C	ALA	852	4.155	46.921	-2.313	1.00	26.66	6
ATOM	255	O	ALA	852	3.957	47.275	-1.154	1.00	26.66	8
ATOM	256	N	ALA	853	5.346	46.931	-2.890	1.00	89.52	7
ATOM	257	CA	ALA	853	6.532	47.410	-2.204	1.00	89.52	6
ATOM	258	CB	ALA	853	7.355	46.243	-1.675	1.00	23.28	6
ATOM	259	C	ALA	853	7.324	48.210	-3.229	1.00	89.52	6
ATOM	260	O	ALA	853	7.765	47.668	-4.240	1.00	89.52	8
ATOM	261	N	ILE	854	7.417	49.467	-3.319	1.00	41.73	7
ATOM	262	CA	ILE	854	8.279	50.444	-3.999	1.00	41.73	6
ATOM	263	CB	ILE	854	7.851	51.866	-3.630	1.00	71.42	6
ATOM	264	CG2	ILE	854	8.539	52.937	-4.479	1.00	83.27	6
ATOM	265	CG1	ILE	854	6.349	52.102	-3.802	1.00	83.27	6
ATOM	266	CD1	ILE	854	5.768	51.388	-5.024	1.00	83.27	6
ATOM	267	C	ILE	854	9.736	50.239	-3.577	1.00	41.73	6
ATOM	268	O	ILE	854	10.035	50.042	-2.390	1.00	41.73	8
ATOM	269	N	LYS	855	10.597	50.294	-4.576	1.00	62.34	7
ATOM	270	CA	LYS	855	12.045	50.123	-4.395	1.00	62.34	6
ATOM	271	CB	LYS	855	12.496	48.792	-5.001	1.00	99.81	6
ATOM	272	CG	LYS	855	13.652	48.147	-4.235	1.00	99.81	6
ATOM	273	CD	LYS	855	13.741	46.635	-4.449	1.00	99.81	6
ATOM	274	CE	LYS	855	13.407	46.212	-5.881	1.00	99.81	6
ATOM	275	NZ	LYS	855	14.507	46.460	-6.824	1.00	99.81	7

FIG. 3E

ATOM	276	C	LYS	855	12.797	51.263	-5.085	1.00	62.34	6
ATOM	277	O	LYS	855	12.216	52.028	-5.869	1.00	62.34	8
ATOM	278	N	ARG	856	14.076	51.334	-4.765	1.00	100.00	7
ATOM	279	CA	ARG	856	14.982	52.353	-5.313	1.00	100.00	6
ATOM	280	CB	ARG	856	14.324	53.733	-5.241	1.00	95.22	6
ATOM	281	CG	ARG	856	15.161	54.829	-5.903	1.00	95.22	6
ATOM	282	CD	ARG	856	14.465	56.192	-5.906	1.00	95.22	6
ATOM	283	NE	ARG	856	15.316	57.271	-6.428	1.00	95.22	7
ATOM	284	CZ	ARG	856	14.938	58.554	-6.503	1.00	95.22	6
ATOM	285	NH1	ARG	856	13.723	58.940	-6.093	1.00	95.22	7
ATOM	286	NH2	ARG	856	15.715	59.537	-6.979	1.00	95.22	7
ATOM	287	C	ARG	856	16.284	52.382	-4.510	1.00	100.00	6
ATOM	288	O	ARG	856	16.269	52.404	-3.270	1.00	100.00	8
ATOM	289	N	MET	857	17.443	52.378	-5.338	1.00	100.00	7
ATOM	290	CA	MET	857	18.288	53.750	-3.743	1.00	100.00	6
ATOM	291	CB	MET	857	18.449	53.097	-2.384	1.00	100.00	6
ATOM	292	CG	MET	857	17.994	54.017	-1.306	1.00	100.00	6
ATOM	293	SD	MET	857	18.352	53.350	0.258	1.00	100.00	16
ATOM	294	CE	MET	857	20.116	53.447	0.204	1.00	100.00	6
ATOM	295	C	MET	857	19.646	53.843	-4.450	1.00	100.00	6
ATOM	296	O	MET	857	20.497	52.937	-4.253	1.00	100.00	8
ATOM	297	OXT	MET	857	19.839	54.838	-5.196	1.00	82.10	8
TER										
ATOM	298	CB	ASP	864	22.499	59.975	-11.088	1.00	55.87	6
ATOM	299	C	ASP	864	23.323	58.318	-12.792	1.00	100.00	6
ATOM	300	O	ASP	864	22.981	58.052	-13.940	1.00	100.00	8
ATOM	301	N	ASP	864	22.263	57.542	-10.688	1.00	100.00	7
ATOM	302	CA	ASP	864	22.263	58.615	-11.734	1.00	100.00	6
ATOM	303	N	ASP	865	24.599	58.333	-12.412	1.00	100.00	7
ATOM	304	CA	ASP	865	25.670	57.988	-13.347	1.00	100.00	6
ATOM	305	CB	ASP	865	26.925	58.842	-13.098	1.00	87.31	6
ATOM	306	C	ASP	865	25.951	56.494	-13.073	1.00	100.00	6
ATOM	307	O	ASP	865	26.537	55.781	-13.902	1.00	100.00	8
ATOM	308	N	HIS	866	25.485	56.080	-11.889	1.00	99.63	7
ATOM	309	CA	HIS	866	25.554	54.713	-11.357	1.00	99.63	6
ATOM	310	CB	HIS	866	25.728	54.726	-9.827	1.00	100.00	6
ATOM	311	CG	HIS	866	24.600	55.378	-9.079	1.00	100.00	6
ATOM	312	CD2	HIS	866	23.472	54.858	-8.543	1.00	100.00	6
ATOM	313	ND1	HIS	866	24.593	56.720	-8.769	1.00	100.00	7
ATOM	314	CE1	HIS	866	23.509	57.002	-8.065	1.00	100.00	6
ATOM	315	NE2	HIS	866	22.811	55.888	-7.915	1.00	100.00	7
ATOM	316	C	HIS	866	24.196	54.120	-11.715	1.00	99.63	6
ATOM	317	O	HIS	866	23.599	53.339	-10.964	1.00	99.63	8
ATOM	318	N	ARG	867	23.732	54.498	-12.904	1.00	100.00	7
ATOM	319	CA	ARG	867	22.419	54.106	-13.405	1.00	100.00	6
ATOM	320	CB	ARG	867	21.700	55.371	-13.954	1.00	100.00	6
ATOM	321	CG	ARG	867	21.971	55.721	-15.445	1.00	100.00	6
ATOM	322	CD	ARG	867	23.460	55.680	-15.790	1.00	100.00	6
ATOM	323	NE	ARG	867	23.698	55.859	-17.219	1.00	100.00	7
ATOM	324	CZ	ARG	867	24.794	55.439	-17.837	1.00	100.00	6
ATOM	325	NH1	ARG	867	25.733	54.810	-17.137	1.00	100.00	7
ATOM	326	NH2	ARG	867	24.940	55.628	-19.145	1.00	100.00	7
ATOM	327	C	ARG	867	22.524	53.015	-14.480	1.00	100.00	6
ATOM	328	O	ARG	867	21.980	53.140	-15.575	1.00	100.00	8
ATOM	329	N	ASP	868	23.225	51.934	-14.164	1.00	100.00	7
ATOM	330	CA	ASP	868	23.393	50.867	-15.146	1.00	100.00	6
ATOM	331	CB	ASP	868	24.591	49.998	-14.773	1.00	100.00	6

FIG. 3F

ATOM	332	CG	ASP	868	24.412	49.314	-13.435	1.00100.00	6
ATOM	333	OD1	ASP	868	24.613	49.980	-12.391	1.00100.00	8
ATOM	334	OD2	ASP	868	24.027	48.130	-13.442	1.00100.00	8
ATOM	335	C	ASP	868	22.154	49.960	-15.282	1.00100.00	6
ATOM	336	O	ASP	868	22.293	48.750	-15.504	1.00100.00	8
ATOM	337	N	PHE	869	20.955	50.538	-15.156	1.00100.00	7
ATOM	338	CA	PHE	869	19.717	49.746	-15.259	1.00100.00	6
ATOM	339	CB	PHE	869	18.424	50.554	-15.017	1.00 99.62	6
ATOM	340	CG	PHE	869	18.595	52.044	-14.986	1.00 99.62	6
ATOM	341	CD1	PHE	869	18.716	52.692	-13.761	1.00 99.62	6
ATOM	342	CD2	PHE	869	18.498	52.813	-16.148	1.00 99.62	6
ATOM	343	CE1	PHE	869	18.734	54.068	-13.681	1.00 99.62	6
ATOM	344	CE2	PHE	869	18.515	54.204	-16.077	1.00 99.62	6
ATOM	345	CZ	PHE	869	18.630	54.834	-14.843	1.00 99.62	6
ATOM	346	C	PHE	869	19.576	49.080	-16.612	1.00100.00	6
ATOM	347	O	PHE	869	20.380	49.305	-17.508	1.00100.00	8
ATOM	348	N	ALA	870	18.524	48.278	-16.746	1.00100.00	7
ATOM	349	CA	ALA	870	18.206	47.512	-17.951	1.00100.00	6
ATOM	350	CB	ALA	870	19.005	48.006	-19.156	1.00 97.10	6
ATOM	351	C	ALA	870	18.532	46.061	-17.670	1.00100.00	6
ATOM	352	O	ALA	870	17.644	45.222	-17.671	1.00100.00	8
ATOM	353	N	GLY	871	19.810	45.775	-17.434	1.00100.00	7
ATOM	354	CA	GLY	871	20.221	44.419	-17.133	1.00100.00	6
ATOM	355	C	GLY	871	19.602	44.044	-15.804	1.00100.00	6
ATOM	356	O	GLY	871	19.400	42.871	-15.506	1.00100.00	8
ATOM	357	N	GLU	872	19.305	45.055	-14.996	1.00 99.97	7
ATOM	358	CA	GLU	872	18.669	44.813	-13.718	1.00 99.97	6
ATOM	359	CB	GLU	872	18.811	46.023	-12.787	1.00100.00	6
ATOM	360	CG	GLU	872	17.496	46.495	-12.182	1.00100.00	6
ATOM	361	CD	GLU	872	17.571	46.692	-10.675	1.00100.00	6
ATOM	362	OE1	GLU	872	18.323	47.585	-10.230	1.00100.00	8
ATOM	363	OE2	GLU	872	16.882	45.946	-9.940	1.00100.00	8
ATOM	364	C	GLU	872	17.200	44.565	-14.033	1.00 99.97	6
ATOM	365	O	GLU	872	16.575	43.673	-13.465	1.00 99.97	8
ATOM	366	N	LEU	873	16.659	45.350	-14.961	1.00 63.02	7
ATOM	367	CA	LEU	873	15.255	45.213	-15.327	1.00 63.02	6
ATOM	368	CB	LEU	873	14.756	46.482	-15.955	1.00 69.97	6
ATOM	369	C	LEU	873	14.977	44.032	-16.243	1.00 63.02	6
ATOM	370	O	LEU	873	13.990	43.323	-16.052	1.00 63.02	8
ATOM	371	N	GLU	874	15.847	43.819	-17.227	1.00100.00	7
ATOM	372	CA	GLU	874	15.687	42.716	-18.164	1.00100.00	6
ATOM	373	CB	GLU	874	16.645	42.862	-19.331	1.00 19.50	6
ATOM	374	C	GLU	874	15.923	41.394	-17.454	1.00100.00	6
ATOM	375	O	GLU	874	15.103	40.482	-17.547	1.00100.00	8
ATOM	376	N	VAL	875	17.040	41.298	-16.737	1.00 69.27	7
ATOM	377	CA	VAL	875	17.383	40.082	-16.002	1.00 69.27	6
ATOM	378	CB	VAL	875	18.763	40.218	-15.359	1.00 39.27	6
ATOM	379	C	VAL	875	16.344	39.755	-14.934	1.00 69.27	6
ATOM	380	O	VAL	875	16.338	38.651	-14.399	1.00 69.27	8
ATOM	381	N	LEU	876	15.493	40.728	-14.613	1.00 78.00	7
ATOM	382	CA	LEU	876	14.438	40.543	-13.616	1.00 78.00	6
ATOM	383	CB	LEU	876	14.169	41.853	-12.843	1.00 53.20	6
ATOM	384	CG	LEU	876	14.939	42.141	-11.537	1.00 29.26	6
ATOM	385	CD1	LEU	876	14.466	43.420	-10.852	1.00 29.26	6
ATOM	386	CD2	LEU	876	14.715	40.969	-10.608	1.00 29.26	6
ATOM	387	C	LEU	876	13.147	40.076	-14.290	1.00 78.00	6
ATOM	388	O	LEU	876	12.410	39.262	-13.737	1.00 78.00	8

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ATOM	389	N	CYS	877	12.870	40.591	-15.486	1.00	60.18	7
ATOM	390	CA	CYS	877	11.652	40.208	-16.191	1.00	60.18	6
ATOM	391	CB	CYS	877	11.199	41.317	-17.164	1.00	100.00	6
ATOM	392	SG	CYS	877	12.370	41.807	-18.447	1.00	100.00	16
ATOM	393	C	CYS	877	11.857	38.886	-16.916	1.00	60.18	6
ATOM	394	O	CYS	877	11.194	38.591	-17.909	1.00	60.18	8
ATOM	395	N	LYS	878	12.788	38.094	-16.398	1.00	65.17	7
ATOM	396	CA	LYS	878	13.088	36.788	-16.964	1.00	65.17	6
ATOM	397	CB	LYS	878	14.593	36.609	-17.078	1.00	89.20	6
ATOM	398	CG	LYS	878	15.190	37.551	-18.092	1.00	52.09	6
ATOM	399	CD	LYS	878	16.693	37.453	-18.128	1.00	52.09	6
ATOM	400	CE	LYS	878	17.289	38.360	-19.216	1.00	52.09	6
ATOM	401	NZ	LYS	878	16.965	37.922	-20.614	1.00	52.09	7
ATOM	402	C	LYS	878	12.473	35.703	-16.091	1.00	65.17	6
ATOM	403	O	LYS	878	12.100	34.632	-16.572	1.00	65.17	8
ATOM	404	N	LEU	879	12.365	35.982	-14.801	1.00	100.00	7
ATOM	405	CA	LEU	879	11.752	35.044	-13.879	1.00	100.00	6
ATOM	406	CB	LEU	879	12.480	35.052	-12.526	1.00	45.22	6
ATOM	407	CG	LEU	879	12.801	36.419	-11.904	1.00	46.30	6
ATOM	408	CD1	LEU	879	13.226	36.250	-10.462	1.00	46.30	6
ATOM	409	CD2	LEU	879	13.892	37.109	-12.704	1.00	46.30	6
ATOM	410	C	LEU	879	10.301	35.492	-13.717	1.00	100.00	6
ATOM	411	O	LEU	879	10.019	36.656	-13.405	1.00	100.00	8
ATOM	412	N	GLY	880	9.381	34.572	-13.972	1.00	96.05	7
ATOM	413	CA	GLY	880	7.980	34.903	-13.848	1.00	96.05	6
ATOM	414	C	GLY	880	7.540	34.784	-12.409	1.00	96.05	6
ATOM	415	O	GLY	880	8.358	34.825	-11.483	1.00	96.05	8
ATOM	416	N	HIS	881	6.236	34.641	-12.216	1.00	70.51	7
ATOM	417	CA	HIS	881	5.693	34.496	-10.876	1.00	70.51	6
ATOM	418	CB	HIS	881	4.178	34.726	-10.843	1.00	99.80	6
ATOM	419	CG	HIS	881	3.498	34.160	-9.629	1.00	99.80	6
ATOM	420	CD2	HIS	881	3.000	32.924	-9.383	1.00	99.80	6
ATOM	421	ND1	HIS	881	3.264	34.897	-8.484	1.00	99.80	7
ATOM	422	CE1	HIS	881	2.648	34.142	-7.592	1.00	99.80	6
ATOM	423	NE2	HIS	881	2.477	32.939	-8.110	1.00	99.80	7
ATOM	424	C	HIS	881	5.952	33.094	-10.384	1.00	70.51	6
ATOM	425	O	HIS	881	5.908	32.134	-11.147	1.00	70.51	8
ATOM	426	N	HIS	882	6.231	32.982	-9.104	1.00	45.83	7
ATOM	427	CA	HIS	882	6.404	31.672	-8.546	1.00	45.83	6
ATOM	428	CB	HIS	882	7.866	31.289	-8.449	1.00	14.81	6
ATOM	429	CG	HIS	882	8.076	29.813	-8.295	1.00	29.81	6
ATOM	430	CD2	HIS	882	7.783	28.782	-9.126	1.00	29.81	6
ATOM	431	ND1	HIS	882	8.608	29.244	-7.167	1.00	29.81	7
ATOM	432	CE1	HIS	882	8.638	27.932	-7.299	1.00	29.81	6
ATOM	433	NE2	HIS	882	8.142	27.626	-8.484	1.00	29.81	7
ATOM	434	C	HIS	882	5.773	31.719	-7.182	1.00	45.83	6
ATOM	435	O	HIS	882	5.987	32.655	-6.411	1.00	45.83	8
ATOM	436	N	PRO	883	4.959	30.711	-6.873	1.00	37.21	7
ATOM	437	CD	PRO	883	4.747	29.405	-7.508	1.00	52.55	6
ATOM	438	CA	PRO	883	4.353	30.762	-5.556	1.00	37.21	6
ATOM	439	CB	PRO	883	3.821	29.336	-5.373	1.00	47.02	6
ATOM	440	CG	PRO	883	4.591	28.493	-6.316	1.00	52.55	6
ATOM	441	C	PRO	883	5.359	31.209	-4.487	1.00	37.21	6
ATOM	442	O	PRO	883	4.990	31.958	-3.579	1.00	37.21	8
ATOM	443	N	ASN	884	6.628	30.800	-4.601	1.00	24.86	7
ATOM	444	CA	ASN	884	7.619	31.198	-3.582	1.00	24.86	6
ATOM	445	CB	ASN	884	8.077	29.996	-2.714	1.00	18.47	6

FIG. 3H

ATOM	446	CG	ASN	884	7.553	28.671	-3.203	1.00	33.47	6
ATOM	447	OD1	ASN	884	7.951	28.205	-4.243	1.00	33.47	8
ATOM	448	ND2	ASN	884	6.674	28.052	-2.443	1.00	33.47	7
ATOM	449	C	ASN	884	8.860	31.986	-4.022	1.00	24.86	6
ATOM	450	O	ASN	884	9.996	31.540	-3.862	1.00	24.86	8
ATOM	451	N	ILE	885	8.603	33.191	-4.518	1.00	46.00	7
ATOM	452	CA	ILE	885	9.616	34.125	-4.986	1.00	46.00	6
ATOM	453	CB	ILE	885	10.063	33.811	-6.435	1.00	25.68	6
ATOM	454	CG2	ILE	885	10.616	35.056	-7.119	1.00	21.87	6
ATOM	455	CG1	ILE	885	11.101	32.696	-6.451	1.00	21.87	6
ATOM	456	CD1	ILE	885	11.855	32.614	-7.727	1.00	21.87	6
ATOM	457	C	ILE	885	8.924	35.476	-5.013	1.00	46.00	6
ATOM	458	O	ILE	885	7.845	35.596	-5.601	1.00	46.00	8
ATOM	459	N	ILE	886	9.501	36.488	-4.373	1.00	36.62	7
ATOM	460	CA	ILE	886	8.857	37.785	-4.434	1.00	36.62	6
ATOM	461	CB	ILE	886	9.462	38.768	-3.414	1.00	17.99	6
ATOM	462	CG2	ILE	886	9.259	40.221	-3.846	1.00	27.09	6
ATOM	463	CG1	ILE	886	8.764	38.531	-2.075	1.00	27.09	6
ATOM	464	CD1	ILE	886	9.230	39.402	-1.000	1.00	27.09	6
ATOM	465	C	ILE	886	8.969	38.250	-5.881	1.00	36.62	6
ATOM	466	O	ILE	886	10.040	38.615	-6.363	1.00	36.62	8
ATOM	467	N	ASN	887	7.832	38.163	-6.566	1.00	39.60	7
ATOM	468	CA	ASN	887	7.716	38.506	-7.975	1.00	39.60	6
ATOM	469	CB	ASN	887	6.531	37.759	-8.603	1.00	82.94	6
ATOM	470	CG	ASN	887	6.602	36.250	-8.406	1.00	82.94	6
ATOM	471	OD1	ASN	887	7.490	35.584	-8.932	1.00	82.94	8
ATOM	472	ND2	ASN	887	5.665	35.710	-7.637	1.00	82.94	7
ATOM	473	C	ASN	887	7.535	39.990	-8.222	1.00	39.60	6
ATOM	474	O	ASN	887	6.893	40.687	-7.432	1.00	39.60	8
ATOM	475	N	LEU	888	8.125	40.438	-9.332	1.00	73.28	7
ATOM	476	CA	LEU	888	8.067	41.822	-9.789	1.00	73.28	6
ATOM	477	CB	LEU	888	9.044	42.055	-10.953	1.00	34.36	6
ATOM	478	CG	LEU	888	9.064	43.390	-11.721	1.00	18.51	6
ATOM	479	CD1	LEU	888	9.760	44.444	-10.873	1.00	18.51	6
ATOM	480	CD2	LEU	888	9.809	43.220	-13.035	1.00	18.51	6
ATOM	481	C	LEU	888	6.651	42.083	-10.274	1.00	73.28	6
ATOM	482	O	LEU	888	6.083	41.282	-11.022	1.00	73.28	8
ATOM	483	N	LEU	889	6.091	43.210	-9.853	1.00	99.59	7
ATOM	484	CA	LEU	889	4.731	43.573	-10.235	1.00	99.59	6
ATOM	485	CB	LEU	889	3.936	43.972	-8.975	1.00	97.88	6
ATOM	486	CG	LEU	889	3.874	42.924	-7.838	1.00	59.80	6
ATOM	487	CD1	LEU	889	2.923	43.357	-6.733	1.00	59.80	6
ATOM	488	CD2	LEU	889	3.419	41.589	-8.413	1.00	59.80	6
ATOM	489	C	LEU	889	4.676	44.676	-11.304	1.00	99.59	6
ATOM	490	O	LEU	889	3.805	44.645	-12.167	1.00	99.59	8
ATOM	491	N	GLY	890	5.599	45.636	-11.266	1.00	54.35	7
ATOM	492	CA	GLY	890	5.597	46.699	-12.264	1.00	54.35	6
ATOM	493	C	GLY	890	6.668	47.737	-11.986	1.00	54.35	6
ATOM	494	O	GLY	890	7.617	47.466	-11.259	1.00	54.35	8
ATOM	495	N	ALA	891	6.534	48.926	-12.560	1.00	66.65	7
ATOM	496	CA	ALA	891	7.515	49.985	-12.328	1.00	66.65	6
ATOM	497	CB	ALA	891	8.872	49.590	-12.911	1.00	68.11	6
ATOM	498	C	ALA	891	7.055	51.299	-12.937	1.00	66.65	6
ATOM	499	O	ALA	891	6.176	51.318	-13.789	1.00	66.65	8
ATOM	500	N	CYS	892	7.656	52.393	-12.485	1.00	99.57	7
ATOM	501	CA	CYS	892	7.322	53.720	-12.984	1.00	99.57	6
ATOM	502	CB	CYS	892	6.872	54.619	-11.833	1.00	98.88	6

FIG. 3I

ATOM	503	SG	CYS	892	5.614	55.803	-12.345	1.00	92.24	16
ATOM	504	C	CYS	892	8.579	54.284	-13.611	1.00	99.57	6
ATOM	505	O	CYS	892	9.610	53.625	-13.607	1.00	99.57	8
ATOM	506	N	GLU	893	8.503	55.485	-14.165	1.00	99.69	7
ATOM	507	CA	GLU	893	9.676	56.130	-14.759	1.00	99.69	6
ATOM	508	CB	GLU	893	9.687	55.991	-16.289	1.00	100.00	6
ATOM	509	CG	GLU	893	10.439	54.776	-16.825	1.00	100.00	6
ATOM	510	CD	GLU	893	10.793	54.883	-18.308	1.00	100.00	6
ATOM	511	OE1	GLU	893	11.715	55.657	-18.646	1.00	100.00	8
ATOM	512	OE2	GLU	893	10.123	54.219	-19.128	1.00	100.00	8
ATOM	513	C	GLU	893	9.616	57.594	-14.387	1.00	99.69	6
ATOM	514	O	GLU	893	9.817	58.469	-15.215	1.00	99.69	8
ATOM	515	N	HIS	894	9.516	57.779	-12.908	1.00	96.96	7
ATOM	516	CA	HIS	894	9.344	59.158	-12.428	1.00	96.96	6
ATOM	517	CB	HIS	894	8.697	59.154	-11.042	1.00	100.00	6
ATOM	518	CG	HIS	894	8.186	60.532	-10.618	1.00	100.00	6
ATOM	519	CD2	HIS	894	7.291	61.381	-11.187	1.00	100.00	6
ATOM	520	ND1	HIS	894	8.631	61.157	-9.457	1.00	100.00	7
ATOM	521	CE1	HIS	894	8.019	62.323	-9.357	1.00	100.00	6
ATOM	522	NE2	HIS	894	7.216	62.472	-10.381	1.00	100.00	7
ATOM	523	C	HIS	894	10.703	59.854	-12.336	1.00	96.96	6
ATOM	524	O	HIS	894	11.756	59.200	-12.319	1.00	96.96	8
ATOM	525	N	ARG	895	10.631	61.171	-12.278	1.00	100.00	7
ATOM	526	CA	ARG	895	11.818	62.033	-12.182	1.00	100.00	6
ATOM	527	CB	ARG	895	11.408	63.440	-11.741	1.00	100.00	6
ATOM	528	CG	ARG	895	10.703	64.230	-12.846	1.00	100.00	6
ATOM	529	CD	ARG	895	10.357	65.661	-12.430	1.00	100.00	6
ATOM	530	NE	ARG	895	10.896	66.673	-13.350	1.00	100.00	7
ATOM	531	CZ	ARG	895	10.138	67.483	-14.101	1.00	100.00	6
ATOM	532	NH1	ARG	895	8.801	67.415	-14.056	1.00	100.00	7
ATOM	533	NH2	ARG	895	10.630	68.406	-14.939	1.00	100.00	7
ATOM	534	C	ARG	895	12.796	61.452	-11.159	1.00	100.00	6
ATOM	535	O	ARG	895	12.399	60.726	-10.236	1.00	100.00	8
ATOM	536	N	GLY	896	14.055	61.795	-11.359	1.00	100.00	7
ATOM	537	CA	GLY	896	15.150	61.337	-10.493	1.00	100.00	6
ATOM	538	C	GLY	896	14.949	59.861	-10.145	1.00	100.00	6
ATOM	539	O	GLY	896	14.575	59.517	-9.013	1.00	100.00	8
ATOM	540	N	TYR	897	15.205	59.037	-11.143	1.00	100.00	7
ATOM	541	CA	TYR	897	15.068	57.578	-11.033	1.00	100.00	6
ATOM	542	CB	TYR	897	15.624	57.096	-9.692	1.00	100.00	6
ATOM	543	CG	TYR	897	15.964	55.604	-9.688	1.00	100.00	6
ATOM	544	CD1	TYR	897	17.195	55.165	-10.192	1.00	100.00	6
ATOM	545	CE1	TYR	897	17.506	53.800	-10.190	1.00	100.00	6
ATOM	546	CD2	TYR	897	15.045	54.676	-9.182	1.00	100.00	6
ATOM	547	CE2	TYR	897	15.357	53.311	-9.179	1.00	100.00	6
ATOM	548	CZ	TYR	897	16.587	52.873	-9.684	1.00	100.00	6
ATOM	549	OH	TYR	897	16.890	51.547	-9.682	1.00	100.00	8
ATOM	550	C	TYR	897	13.592	57.190	-11.131	1.00	100.00	6
ATOM	551	O	TYR	897	12.714	58.051	-11.293	1.00	100.00	8
ATOM	552	N	LEU	898	13.367	55.894	-11.027	1.00	100.00	7
ATOM	553	CA	LEU	898	12.020	55.310	-11.093	1.00	100.00	6
ATOM	554	CB	LEU	898	11.960	54.258	-12.202	1.00	41.85	6
ATOM	555	C	LEU	898	11.672	54.648	-9.759	1.00	100.00	6
ATOM	556	O	LEU	898	12.234	54.992	-8.709	1.00	100.00	8
ATOM	557	N	TYR	899	10.747	53.711	-9.850	1.00	72.77	7
ATOM	558	CA	TYR	899	10.267	52.951	-8.688	1.00	72.77	6
ATOM	559	CB	TYR	899	9.153	53.725	-7.982	1.00	100.00	6

FIG. 3J

ATOM	560	CG	TYR	899	9.685	54.728	-6.958	1.00100.00	6
ATOM	561	CD1	TYR	899	9.394	56.090	-7.096	1.00100.00	6
ATOM	562	CE1	TYR	899	9.884	57.008	-6.159	1.00100.00	6
ATOM	563	CD2	TYR	899	10.465	54.283	-5.884	1.00100.00	6
ATOM	564	CE2	TYR	899	10.955	55.201	-4.948	1.00100.00	6
ATOM	565	CZ	TYR	899	10.664	56.564	-5.085	1.00100.00	6
ATOM	566	OH	TYR	899	11.140	57.456	-4.175	1.00100.00	8
ATOM	567	C	TYR	899	9.726	51.592	-9.136	1.00 72.77	6
ATOM	568	O	TYR	899	8.785	51.513	-9.940	1.00 72.77	8
ATOM	569	N	LEU	900	10.350	50.565	-8.591	1.00 78.27	7
ATOM	570	CA	LEU	900	9.996	49.168	-8.876	1.00 78.27	6
ATOM	571	CB	LEU	900	11.233	48.277	-8.738	1.00 79.18	6
ATOM	572	CG	LEU	900	11.566	47.512	-10.020	1.00 54.43	6
ATOM	573	CD1	LEU	900	11.602	48.408	-11.259	1.00 54.43	6
ATOM	574	CD2	LEU	900	12.931	46.823	-9.967	1.00 54.43	6
ATOM	575	C	LEU	900	8.927	48.689	-7.892	1.00 78.27	6
ATOM	576	O	LEU	900	9.079	48.823	-6.669	1.00 78.27	8
ATOM	577	N	ALA	901	7.874	48.141	-8.468	1.00 72.23	7
ATOM	578	CA	ALA	901	6.731	47.614	-7.708	1.00 72.23	6
ATOM	579	CB	ALA	901	5.424	47.944	-8.433	1.00 33.79	6
ATOM	580	C	ALA	901	6.851	46.095	-7.568	1.00 72.23	6
ATOM	581	O	ALA	901	7.121	45.383	-8.546	1.00 72.23	8
ATOM	582	N	ILE	902	6.929	45.582	-6.293	1.00 59.87	7
ATOM	583	CA	ILE	902	7.104	44.154	-6.059	1.00 59.87	6
ATOM	584	CB	ILE	902	8.550	43.900	-5.623	1.00 34.80	6
ATOM	585	CG2	ILE	902	9.522	44.289	-6.729	1.00 35.77	6
ATOM	586	CG1	ILE	902	8.846	44.755	-4.397	1.00 35.77	6
ATOM	587	CD1	ILE	902	10.311	45.018	-4.169	1.00 35.77	6
ATOM	588	C	ILE	902	6.165	43.633	-4.969	1.00 59.87	6
ATOM	589	O	ILE	902	5.750	44.390	-4.093	1.00 59.87	8
ATOM	590	N	GLU	903	5.835	42.344	-5.030	1.00 34.73	7
ATOM	591	CA	GLU	903	4.967	41.716	-4.036	1.00 34.73	6
ATOM	592	CB	GLU	903	5.047	40.197	-4.119	1.00 38.01	6
ATOM	593	CG	GLU	903	4.180	39.568	-5.170	1.00 49.25	6
ATOM	594	CD	GLU	903	4.216	38.043	-5.112	1.00 49.25	6
ATOM	595	OE1	GLU	903	4.310	37.497	-3.985	1.00 49.25	8
ATOM	596	OE2	GLU	903	4.141	37.403	-6.191	1.00 49.25	8
ATOM	597	C	GLU	903	5.343	42.124	-2.627	1.00 34.73	6
ATOM	598	O	GLU	903	6.514	42.378	-2.330	1.00 34.73	8
ATOM	599	N	TYR	904	4.328	42.169	-1.770	1.00 31.03	7
ATOM	600	CA	TYR	904	4.469	42.530	-0.370	1.00 31.03	6
ATOM	601	CB	TYR	904	3.411	43.577	-0.003	1.00 13.64	6
ATOM	602	CG	TYR	904	3.419	43.950	1.459	1.00 23.21	6
ATOM	603	CD1	TYR	904	4.598	44.344	2.086	1.00 23.21	6
ATOM	604	CE1	TYR	904	4.647	44.606	3.448	1.00 23.21	6
ATOM	605	CD2	TYR	904	2.276	43.840	2.236	1.00 23.21	6
ATOM	606	CE2	TYR	904	2.315	44.102	3.608	1.00 23.21	6
ATOM	607	CZ	TYR	904	3.509	44.477	4.204	1.00 23.21	6
ATOM	608	OH	TYR	904	3.575	44.663	5.569	1.00 23.21	8
ATOM	609	C	TYR	904	4.328	41.291	0.532	1.00 31.03	6
ATOM	610	O	TYR	904	3.388	40.494	0.393	1.00 31.03	8
ATOM	611	N	ALA	905	5.284	41.154	1.447	1.00 31.20	7
ATOM	612	CA	ALA	905	5.334	40.063	2.409	1.00 31.20	6
ATOM	613	CB	ALA	905	6.733	39.460	2.430	1.00 28.71	6
ATOM	614	C	ALA	905	4.990	40.633	3.781	1.00 31.20	6
ATOM	615	O	ALA	905	5.853	41.091	4.514	1.00 31.20	8
ATOM	616	N	PRO	906	3.716	40.600	4.151	1.00 17.48	7

FIG. 3K

ATOM	617	CD	PRO	906	2.597	40.048	3.370	1.00	32.19	6
ATOM	618	CA	PRO	906	3.241	41.121	5.427	1.00	17.48	6
ATOM	619	CB	PRO	906	1.728	40.964	5.314	1.00	32.19	6
ATOM	620	CG	PRO	906	1.580	39.762	4.442	1.00	32.19	6
ATOM	621	C	PRO	906	3.774	40.564	6.724	1.00	17.48	6
ATOM	622	O	PRO	906	3.408	41.072	7.788	1.00	17.48	8
ATOM	623	N	HIS	907	4.636	39.550	6.683	1.00	30.66	7
ATOM	624	CA	HIS	907	5.123	38.987	7.954	1.00	30.66	6
ATOM	625	CB	HIS	907	4.657	37.543	8.130	1.00	5.00	6
ATOM	626	CG	HIS	907	3.174	37.357	8.048	1.00	5.00	6
ATOM	627	CD2	HIS	907	2.219	37.353	9.011	1.00	5.00	6
ATOM	628	ND1	HIS	907	2.517	37.103	6.865	1.00	5.00	7
ATOM	629	CE1	HIS	907	1.224	36.945	7.097	1.00	5.00	6
ATOM	630	NE2	HIS	907	1.021	37.091	8.393	1.00	5.00	7
ATOM	631	C	HIS	907	6.622	39.004	8.229	1.00	30.66	6
ATOM	632	O	HIS	907	7.130	38.115	8.926	1.00	30.66	8
ATOM	633	N	GLY	908	7.326	40.009	7.718	1.00	38.98	7
ATOM	634	CA	GLY	908	8.756	40.081	7.947	1.00	38.98	6
ATOM	635	C	GLY	908	9.483	38.924	7.298	1.00	38.98	6
ATOM	636	O	GLY	908	8.935	38.235	6.436	1.00	38.98	8
ATOM	637	N	ASN	909	10.719	38.698	7.718	1.00	31.42	7
ATOM	638	CA	ASN	909	11.517	37.620	7.140	1.00	31.42	6
ATOM	639	CB	ASN	909	12.963	38.068	6.941	1.00	41.70	6
ATOM	640	CG	ASN	909	13.566	38.630	8.197	1.00	41.70	6
ATOM	641	OD1	ASN	909	14.196	39.684	8.168	1.00	41.70	8
ATOM	642	ND2	ASN	909	13.381	37.931	9.316	1.00	41.70	7
ATOM	643	C	ASN	909	11.488	36.349	7.964	1.00	31.42	6
ATOM	644	O	ASN	909	11.094	36.340	9.132	1.00	31.42	8
ATOM	645	N	LEU	910	11.937	35.275	7.347	1.00	17.12	7
ATOM	646	CA	LEU	910	11.930	34.014	8.019	1.00	17.12	6
ATOM	647	CB	LEU	910	12.524	32.962	7.139	1.00	20.29	6
ATOM	648	CG	LEU	910	12.192	31.558	7.604	1.00	20.29	6
ATOM	649	CD1	LEU	910	10.687	31.274	7.677	1.00	20.29	6
ATOM	650	CD2	LEU	910	12.850	30.696	6.590	1.00	20.29	6
ATOM	651	C	LEU	910	12.679	34.039	9.332	1.00	17.12	6
ATOM	652	O	LEU	910	12.183	33.554	10.355	1.00	17.12	8
ATOM	653	N	LEU	911	13.885	34.579	9.319	1.00	21.04	7
ATOM	654	CA	LEU	911	14.646	34.644	10.551	1.00	21.04	6
ATOM	655	CB	LEU	911	15.865	35.523	10.363	1.00	23.99	6
ATOM	656	CG	LEU	911	16.744	35.463	11.596	1.00	23.99	6
ATOM	657	CD1	LEU	911	17.326	34.053	11.797	1.00	23.99	6
ATOM	658	CD2	LEU	911	17.833	36.483	11.399	1.00	23.99	6
ATOM	659	C	LEU	911	13.791	35.199	11.697	1.00	21.04	6
ATOM	660	O	LEU	911	13.565	34.515	12.692	1.00	21.04	8
ATOM	661	N	ASP	912	13.305	36.429	11.557	1.00	16.81	7
ATOM	662	CA	ASP	912	12.489	37.041	12.618	1.00	16.81	6
ATOM	663	CB	ASP	912	11.973	38.399	12.177	1.00	39.39	6
ATOM	664	CG	ASP	912	12.996	39.463	12.327	1.00	39.39	6
ATOM	665	OD1	ASP	912	12.794	40.557	11.777	1.00	39.39	8
ATOM	666	OD2	ASP	912	14.005	39.185	12.989	1.00	39.39	8
ATOM	667	C	ASP	912	11.311	36.214	13.031	1.00	16.81	6
ATOM	668	O	ASP	912	11.020	36.079	14.215	1.00	16.81	8
ATOM	669	N	PHE	913	10.623	35.698	12.027	1.00	39.11	7
ATOM	670	CA	PHE	913	9.462	34.884	12.255	1.00	39.11	6
ATOM	671	CB	PHE	913	8.850	34.495	10.937	1.00	34.21	6
ATOM	672	CG	PHE	913	7.458	34.005	11.055	1.00	34.21	6
ATOM	673	CD1	PHE	913	6.412	34.897	11.233	1.00	34.21	6

FIG. 3L

ATOM	674	CD2	PHE	913	7.181	32.647	10.986	1.00	34.21	6
ATOM	675	CE1	PHE	913	5.109	34.450	11.343	1.00	34.21	6
ATOM	676	CE2	PHE	913	5.885	32.185	11.094	1.00	34.21	6
ATOM	677	CZ	PHE	913	4.843	33.089	11.271	1.00	34.21	6
ATOM	678	C	PHE	913	9.846	33.636	13.026	1.00	39.11	6
ATOM	679	O	PHE	913	9.073	33.166	13.843	1.00	39.11	8
ATOM	680	N	LEU	914	11.018	33.076	12.770	1.00	29.14	7
ATOM	681	CA	LEU	914	11.389	31.895	13.527	1.00	29.14	6
ATOM	682	CB	LEU	914	12.622	31.212	12.916	1.00	10.91	6
ATOM	683	CG	LEU	914	12.407	30.445	11.606	1.00	10.91	6
ATOM	684	CD1	LEU	914	13.709	29.936	11.066	1.00	10.91	6
ATOM	685	CD2	LEU	914	11.430	29.310	11.861	1.00	10.91	6
ATOM	686	C	LEU	914	11.659	32.247	14.994	1.00	29.14	6
ATOM	687	O	LEU	914	11.215	31.551	15.893	1.00	29.14	8
ATOM	688	N	ARG	915	12.377	33.337	15.228	1.00	18.56	7
ATOM	689	CA	ARG	915	12.750	33.766	16.569	1.00	18.56	6
ATOM	690	CB	ARG	915	13.829	34.844	16.463	1.00	29.12	6
ATOM	691	CG	ARG	915	15.088	34.300	15.887	1.00	29.12	6
ATOM	692	CD	ARG	915	16.140	35.354	15.729	1.00	29.12	6
ATOM	693	NE	ARG	915	17.459	34.736	15.660	1.00	29.12	7
ATOM	694	CZ	ARG	915	18.580	35.352	15.285	1.00	29.12	6
ATOM	695	NH1	ARG	915	18.545	36.630	14.924	1.00	29.12	7
ATOM	696	NH2	ARG	915	19.745	34.689	15.287	1.00	29.12	7
ATOM	697	C	ARG	915	11.609	34.256	17.439	1.00	18.56	6
ATOM	698	O	ARG	915	11.641	34.094	18.665	1.00	18.56	8
ATOM	699	N	LYS	916	10.605	34.841	16.788	1.00	22.66	7
ATOM	700	CA	LYS	916	9.426	35.406	17.441	1.00	22.66	6
ATOM	701	CB	LYS	916	8.816	36.463	16.501	1.00	51.60	6
ATOM	702	CG	LYS	916	7.369	36.228	16.021	1.00	51.60	6
ATOM	703	CD	LYS	916	7.163	34.999	15.123	1.00	51.60	6
ATOM	704	CE	LYS	916	5.699	34.865	14.684	1.00	51.60	6
ATOM	705	NZ	LYS	916	4.772	34.565	15.811	1.00	51.60	7
ATOM	706	C	LYS	916	8.377	34.360	17.848	1.00	22.66	6
ATOM	707	O	LYS	916	7.332	34.718	18.366	1.00	22.66	8
ATOM	708	N	SER	917	8.677	33.082	17.633	1.00	22.66	7
ATOM	709	CA	SER	917	7.773	31.979	17.957	1.00	22.66	6
ATOM	710	CB	SER	917	7.623	31.070	16.741	1.00	19.58	6
ATOM	711	OG	SER	917	8.890	30.564	16.328	1.00	19.58	8
ATOM	712	C	SER	917	8.272	31.143	19.135	1.00	22.66	6
ATOM	713	O	SER	917	7.720	30.078	19.436	1.00	22.66	8
ATOM	714	N	ARG	918	9.339	31.602	19.780	1.00	32.97	7
ATOM	715	CA	ARG	918	9.906	30.908	20.934	1.00	32.97	6
ATOM	716	CB	ARG	918	11.372	31.305	21.132	1.00	9.93	6
ATOM	717	CG	ARG	918	12.287	31.089	19.973	1.00	9.93	6
ATOM	718	CD	ARG	918	13.751	31.230	20.402	1.00	9.93	6
ATOM	719	NE	ARG	918	14.633	30.604	19.413	1.00	9.93	7
ATOM	720	CZ	ARG	918	15.957	30.509	19.504	1.00	9.93	6
ATOM	721	NH1	ARG	918	16.610	31.007	20.533	1.00	9.93	7
ATOM	722	NH2	ARG	918	16.637	29.872	18.565	1.00	9.93	7
ATOM	723	C	ARG	918	9.110	31.323	22.177	1.00	32.97	6
ATOM	724	O	ARG	918	9.547	32.189	22.925	1.00	32.97	8
ATOM	725	N	VAL	919	7.943	30.704	22.365	1.00	29.42	7
ATOM	726	CA	VAL	919	7.026	30.973	23.484	1.00	29.42	6
ATOM	727	CB	VAL	919	5.878	29.970	23.518	1.00	31.60	6
ATOM	728	CG1	VAL	919	4.650	30.613	24.113	1.00	31.60	6
ATOM	729	CG2	VAL	919	5.620	29.426	22.134	1.00	31.60	6
ATOM	730	C	VAL	919	7.635	30.893	24.867	1.00	29.42	6

FIG. 3M

ATOM	731	O	VAL	919	7.173	31.537	25.793	1.00	29.42	8
ATOM	732	N	LEU	920	8.635	30.048	25.020	1.00	34.37	7
ATOM	733	CA	LEU	920	9.260	29.900	26.305	1.00	34.37	6
ATOM	734	CB	LEU	920	10.093	28.629	26.324	1.00	36.03	6
ATOM	735	CG	LEU	920	10.688	28.310	27.688	1.00	36.03	6
ATOM	736	CD1	LEU	920	9.559	28.061	28.676	1.00	36.03	6
ATOM	737	CD2	LEU	920	11.592	27.104	27.587	1.00	36.03	6
ATOM	738	C	LEU	920	10.138	31.117	26.552	1.00	34.37	6
ATOM	739	O	LEU	920	10.523	31.393	27.676	1.00	34.37	8
ATOM	740	N	GLU	921	10.472	31.851	25.503	1.00	29.12	7
ATOM	741	CA	GLU	921	11.301	33.025	25.693	1.00	29.12	6
ATOM	742	CB	GLU	921	12.215	33.237	24.485	1.00	99.98	6
ATOM	743	CG	GLU	921	13.435	34.081	24.798	1.00	99.98	6
ATOM	744	CD	GLU	921	13.165	35.574	24.753	1.00	99.98	6
ATOM	745	OE1	GLU	921	12.935	36.086	23.638	1.00	99.98	8
ATOM	746	OE2	GLU	921	13.156	36.228	25.824	1.00	99.98	8
ATOM	747	C	GLU	921	10.362	34.207	25.885	1.00	29.12	6
ATOM	748	O	GLU	921	10.452	34.929	26.869	1.00	29.12	8
ATOM	749	N	THR	922	9.455	34.375	24.932	1.00	52.74	7
ATOM	750	CA	THR	922	8.463	35.437	24.944	1.00	52.74	6
ATOM	751	CB	THR	922	7.450	35.207	23.800	1.00	53.34	6
ATOM	752	OG1	THR	922	8.038	35.598	22.558	1.00	53.34	8
ATOM	753	CG2	THR	922	6.167	35.977	24.026	1.00	53.34	6
ATOM	754	C	THR	922	7.706	35.498	26.265	1.00	52.74	6
ATOM	755	O	THR	922	7.923	36.398	27.077	1.00	52.74	8
ATOM	756	N	ASP	923	6.827	34.515	26.461	1.00	32.25	7
ATOM	757	CA	ASP	923	5.981	34.391	27.651	1.00	32.25	6
ATOM	758	CB	ASP	923	4.509	34.434	27.231	1.00	60.93	6
ATOM	759	CG	ASP	923	3.558	34.328	28.404	1.00	60.93	6
ATOM	760	OD1	ASP	923	3.762	35.032	29.415	1.00	60.93	8
ATOM	761	OD2	ASP	923	2.593	33.545	28.309	1.00	60.93	8
ATOM	762	C	ASP	923	6.295	33.083	28.361	1.00	32.25	6
ATOM	763	O	ASP	923	5.711	32.034	28.055	1.00	32.25	8
ATOM	764	N	PRO	924	7.216	33.146	29.346	1.00	33.34	7
ATOM	765	CD	PRO	924	7.426	34.381	30.130	1.00	100.00	6
ATOM	766	CA	PRO	924	7.637	31.978	30.125	1.00	33.34	6
ATOM	767	CB	PRO	924	8.263	32.605	31.366	1.00	100.00	6
ATOM	768	CG	PRO	924	7.488	33.863	31.535	1.00	100.00	6
ATOM	769	C	PRO	924	6.464	31.030	30.456	1.00	33.34	6
ATOM	770	O	PRO	924	6.470	29.873	30.053	1.00	33.34	8
ATOM	771	N	ALA	925	5.460	31.543	31.164	1.00	69.10	7
ATOM	772	CA	ALA	925	4.282	30.781	31.603	1.00	69.10	6
ATOM	773	CB	ALA	925	3.311	31.735	32.255	1.00	73.73	6
ATOM	774	C	ALA	925	3.562	29.976	30.531	1.00	69.10	6
ATOM	775	O	ALA	925	3.802	28.779	30.384	1.00	69.10	8
ATOM	776	N	PHE	926	2.662	30.639	29.806	1.00	48.64	7
ATOM	777	CA	PHE	926	1.877	30.013	28.743	1.00	48.64	6
ATOM	778	CB	PHE	926	1.766	30.975	27.558	1.00	37.88	6
ATOM	779	CG	PHE	926	0.669	30.632	26.605	1.00	37.88	6
ATOM	780	CD1	PHE	926	-0.646	30.983	26.893	1.00	37.88	6
ATOM	781	CD2	PHE	926	0.926	29.853	25.479	1.00	37.88	6
ATOM	782	CE1	PHE	926	-1.679	30.560	26.089	1.00	37.88	6
ATOM	783	CE2	PHE	926	-0.106	29.420	24.668	1.00	37.88	6
ATOM	784	CZ	PHE	926	-1.406	29.774	24.977	1.00	37.88	6
ATOM	785	C	PHE	926	2.439	28.673	28.267	1.00	48.64	6
ATOM	786	O	PHE	926	1.752	27.656	28.298	1.00	48.64	8
ATOM	787	N	ALA	927	3.688	28.681	27.812	1.00	47.80	7

FIG. 3N

ATOM	788	CA	ALA	927	4.337	27.467	27.340	1.00	47.80	6
ATOM	789	CB	ALA	927	5.786	27.752	26.970	1.00	31.97	6
ATOM	790	C	ALA	927	4.272	26.297	28.314	1.00	47.80	6
ATOM	791	O	ALA	927	3.725	25.256	27.984	1.00	47.80	8
ATOM	792	N	ILE	928	4.850	26.439	29.499	1.00	44.35	7
ATOM	793	CA	ILE	928	4.810	25.346	30.457	1.00	44.35	6
ATOM	794	CB	ILE	928	5.155	25.837	31.868	1.00	67.81	6
ATOM	795	CG2	ILE	928	5.834	24.735	32.641	1.00	29.96	6
ATOM	796	CG1	ILE	928	6.130	27.004	31.806	1.00	29.96	6
ATOM	797	CD1	ILE	928	7.542	26.594	31.485	1.00	29.96	6
ATOM	798	C	ILE	928	3.410	24.718	30.494	1.00	44.35	6
ATOM	799	O	ILE	928	3.266	23.499	30.626	1.00	44.35	8
ATOM	800	N	ALA	929	2.390	25.562	30.346	1.00	42.29	7
ATOM	801	CA	ALA	929	0.984	25.135	30.390	1.00	42.29	6
ATOM	802	CB	ALA	929	0.118	26.315	30.676	1.00	5.26	6
ATOM	803	C	ALA	929	0.457	24.440	29.156	1.00	42.29	6
ATOM	804	O	ALA	929	-0.225	23.429	29.252	1.00	42.29	8
ATOM	805	N	ASN	930	0.745	24.995	27.994	1.00	36.17	7
ATOM	806	CA	ASN	930	0.259	24.398	26.775	1.00	36.17	6
ATOM	807	CB	ASN	930	-0.230	25.506	25.852	1.00	57.20	6
ATOM	808	CG	ASN	930	-1.444	26.223	26.430	1.00	57.20	6
ATOM	809	OD1	ASN	930	-2.586	25.742	26.344	1.00	57.20	8
ATOM	810	ND2	ASN	930	-1.202	27.360	27.057	1.00	57.20	7
ATOM	811	C	ASN	930	1.295	23.486	26.128	1.00	36.17	6
ATOM	812	O	ASN	930	1.088	22.976	25.028	1.00	36.17	8
ATOM	813	N	SER	931	2.401	23.259	26.834	1.00	50.28	7
ATOM	814	CA	SER	931	3.468	22.383	26.353	1.00	50.28	6
ATOM	815	CB	SER	931	2.986	20.930	26.341	1.00	90.81	6
ATOM	816	OG	SER	931	2.790	20.433	27.659	1.00	90.81	8
ATOM	817	C	SER	931	4.006	22.748	24.979	1.00	50.28	6
ATOM	818	O	SER	931	4.484	21.889	24.258	1.00	50.28	8
ATOM	819	N	THR	932	3.918	24.023	24.622	1.00	48.32	7
ATOM	820	CA	THR	932	4.397	24.510	23.334	1.00	48.32	6
ATOM	821	CB	THR	932	3.443	25.591	22.749	1.00	79.61	6
ATOM	822	OG1	THR	932	3.247	26.634	23.711	1.00	79.61	8
ATOM	823	CG2	THR	932	2.108	24.989	22.374	1.00	79.61	6
ATOM	824	C	THR	932	5.784	25.127	23.483	1.00	48.32	6
ATOM	825	O	THR	932	6.046	25.841	24.449	1.00	48.32	8
ATOM	826	N	ALA	933	6.667	24.854	22.527	1.00	55.05	7
ATOM	827	CA	ALA	933	8.009	25.436	22.552	1.00	55.05	6
ATOM	828	CB	ALA	933	9.057	24.378	22.297	1.00	28.55	6
ATOM	829	C	ALA	933	8.051	26.489	21.461	1.00	55.05	6
ATOM	830	O	ALA	933	8.936	27.339	21.437	1.00	55.05	8
ATOM	831	N	SER	934	7.098	26.393	20.543	1.00	27.13	7
ATOM	832	CA	SER	934	6.978	27.340	19.469	1.00	27.13	6
ATOM	833	CB	SER	934	7.937	27.003	18.341	1.00	36.98	6
ATOM	834	OG	SER	934	7.630	27.748	17.167	1.00	36.98	8
ATOM	835	C	SER	934	5.552	27.315	18.959	1.00	27.13	6
ATOM	836	O	SER	934	4.897	26.270	19.001	1.00	27.13	8
ATOM	837	N	THR	935	5.080	28.468	18.488	1.00	15.04	7
ATOM	838	CA	THR	935	3.740	28.582	17.963	1.00	15.04	6
ATOM	839	CB	THR	935	3.387	30.101	17.642	1.00	26.85	6
ATOM	840	OG1	THR	935	4.301	30.658	16.680	1.00	26.85	8
ATOM	841	CG2	THR	935	3.432	30.930	18.917	1.00	26.85	6
ATOM	842	C	THR	935	3.652	27.696	16.712	1.00	15.04	6
ATOM	843	O	THR	935	2.594	27.154	16.407	1.00	15.04	8
ATOM	844	N	LEU	936	4.778	27.530	16.015	1.00	41.56	7

FIG. 30

ATOM	845	CA	LEU	936	4.839	26.720	14.788	1.00	41.56	6
ATOM	846	CB	LEU	936	6.005	27.210	13.915	1.00	16.11	6
ATOM	847	CG	LEU	936	5.980	28.713	13.613	1.00	16.11	6
ATOM	848	CD1	LEU	936	7.108	29.067	12.679	1.00	16.11	6
ATOM	849	CD2	LEU	936	4.640	29.083	13.020	1.00	16.11	6
ATOM	850	C	LEU	936	4.958	25.203	15.018	1.00	41.56	6
ATOM	851	O	LEU	936	5.433	24.744	16.063	1.00	41.56	8
ATOM	852	N	SER	937	4.524	24.440	14.021	1.00	27.35	7
ATOM	853	CA	SER	937	4.551	22.989	14.081	1.00	27.35	6
ATOM	854	CB	SER	937	3.167	22.438	13.764	1.00	9.94	6
ATOM	855	OG	SER	937	2.884	22.429	12.374	1.00	9.94	8
ATOM	856	C	SER	937	5.574	22.357	13.128	1.00	27.35	6
ATOM	857	O	SER	937	6.180	23.041	12.291	1.00	27.35	8
ATOM	858	N	SER	938	5.752	21.043	13.257	1.00	23.83	7
ATOM	859	CA	SER	938	6.689	20.294	12.431	1.00	23.83	6
ATOM	860	CB	SER	938	6.678	18.813	12.838	1.00	31.90	6
ATOM	861	OG	SER	938	7.011	17.966	11.741	1.00	31.90	8
ATOM	862	C	SER	938	6.362	20.431	10.943	1.00	23.83	6
ATOM	863	O	SER	938	7.256	20.590	10.121	1.00	23.83	8
ATOM	864	N	GLN	939	5.083	20.382	10.597	1.00	34.70	7
ATOM	865	CA	GLN	939	4.704	20.491	9.206	1.00	34.70	6
ATOM	866	CB	GLN	939	3.296	19.955	9.022	1.00	40.81	6
ATOM	867	CG	GLN	939	3.189	18.544	9.538	1.00	40.81	6
ATOM	868	CD	GLN	939	4.026	17.558	8.732	1.00	40.81	6
ATOM	869	OE1	GLN	939	3.584	17.084	7.675	1.00	40.81	8
ATOM	870	NE2	GLN	939	5.243	17.254	9.216	1.00	40.81	7
ATOM	871	C	GLN	939	4.838	21.906	8.685	1.00	34.70	6
ATOM	872	O	GLN	939	5.352	22.096	7.592	1.00	34.70	8
ATOM	873	N	GLN	940	4.388	22.906	9.435	1.00	22.70	7
ATOM	874	CA	GLN	940	4.556	24.267	8.950	1.00	22.70	6
ATOM	875	CB	GLN	940	4.094	25.286	9.986	1.00	30.92	6
ATOM	876	CG	GLN	940	4.588	26.679	9.679	1.00	30.92	6
ATOM	877	CD	GLN	940	3.663	27.483	8.790	1.00	30.92	6
ATOM	878	OE1	GLN	940	2.738	28.141	9.277	1.00	30.92	8
ATOM	879	NE2	GLN	940	3.891	27.427	7.482	1.00	30.92	7
ATOM	880	C	GLN	940	6.047	24.501	8.632	1.00	22.70	6
ATOM	881	O	GLN	940	6.381	25.050	7.574	1.00	22.70	8
ATOM	882	N	LEU	941	6.934	24.076	9.535	1.00	22.33	7
ATOM	883	CA	LEU	941	8.377	24.242	9.348	1.00	22.33	6
ATOM	884	CB	LEU	941	9.137	23.858	10.599	1.00	19.37	6
ATOM	885	CG	LEU	941	8.939	24.738	11.806	1.00	19.37	6
ATOM	886	CD1	LEU	941	9.540	23.981	12.995	1.00	19.37	6
ATOM	887	CD2	LEU	941	9.613	26.094	11.606	1.00	19.37	6
ATOM	888	C	LEU	941	8.956	23.427	8.202	1.00	22.33	6
ATOM	889	O	LEU	941	9.994	23.781	7.648	1.00	22.33	8
ATOM	890	N	LEU	942	8.334	22.308	7.869	1.00	30.49	7
ATOM	891	CA	LEU	942	8.877	21.545	6.765	1.00	30.49	6
ATOM	892	CB	LEU	942	8.370	20.098	6.748	1.00	27.17	6
ATOM	893	CG	LEU	942	8.901	19.138	7.816	1.00	27.17	6
ATOM	894	CD1	LEU	942	8.244	17.799	7.576	1.00	27.17	6
ATOM	895	CD2	LEU	942	10.399	18.997	7.776	1.00	27.17	6
ATOM	896	C	LEU	942	8.445	22.285	5.517	1.00	30.49	6
ATOM	897	O	LEU	942	9.211	22.408	4.582	1.00	30.49	8
ATOM	898	N	HIS	943	7.224	22.805	5.502	1.00	24.87	7
ATOM	899	CA	HIS	943	6.766	23.543	4.331	1.00	24.87	6
ATOM	900	CB	HIS	943	5.393	24.127	4.565	1.00	75.69	6
ATOM	901	CG	HIS	943	4.306	23.142	4.316	1.00	75.69	6

FIG. 3P

ATOM	902	CD2	HIS	943	3.224	23.187	3.507	1.00	75.69	6
ATOM	903	ND1	HIS	943	4.317	21.892	4.884	1.00	75.69	7
ATOM	904	CE1	HIS	943	3.284	21.198	4.431	1.00	75.69	6
ATOM	905	NE2	HIS	943	2.608	21.960	3.596	1.00	75.69	7
ATOM	906	C	HIS	943	7.727	24.644	3.967	1.00	24.87	6
ATOM	907	O	HIS	943	8.112	24.794	2.815	1.00	24.87	8
ATOM	908	N	PHE	944	8.107	25.412	4.976	1.00	23.28	7
ATOM	909	CA	PHE	944	9.049	26.499	4.812	1.00	23.28	6
ATOM	910	CB	PHE	944	9.379	27.069	6.196	1.00	24.44	6
ATOM	911	CG	PHE	944	8.293	27.953	6.782	1.00	24.44	6
ATOM	912	CD1	PHE	944	8.361	28.370	8.101	1.00	24.44	6
ATOM	913	CD2	PHE	944	7.282	28.477	5.983	1.00	24.44	6
ATOM	914	CE1	PHE	944	7.449	29.299	8.598	1.00	24.44	6
ATOM	915	CE2	PHE	944	6.372	29.406	6.489	1.00	24.44	6
ATOM	916	CZ	PHE	944	6.466	29.815	7.792	1.00	24.44	6
ATOM	917	C	PHE	944	10.301	26.011	4.079	1.00	23.28	6
ATOM	918	O	PHE	944	10.778	26.675	3.164	1.00	23.28	8
ATOM	919	N	ALA	945	10.829	24.855	4.470	1.00	15.27	7
ATOM	920	CA	ALA	945	11.996	24.310	3.799	1.00	15.27	6
ATOM	921	CB	ALA	945	12.627	23.197	4.645	1.00	55.81	6
ATOM	922	C	ALA	945	11.644	23.804	2.386	1.00	15.27	6
ATOM	923	O	ALA	945	12.493	23.819	1.517	1.00	15.27	8
ATOM	924	N	ALA	946	10.408	23.368	2.139	1.00	9.68	7
ATOM	925	CA	ALA	946	10.011	22.897	0.795	1.00	9.68	6
ATOM	926	CB	ALA	946	8.734	22.042	0.869	1.00	20.69	6
ATOM	927	C	ALA	946	9.760	24.088	-0.114	1.00	9.68	6
ATOM	928	O	ALA	946	10.026	24.032	-1.319	1.00	9.68	8
ATOM	929	N	ASP	947	9.205	25.149	0.471	1.00	24.26	7
ATOM	930	CA	ASP	947	8.922	26.379	-0.245	1.00	24.26	6
ATOM	931	CB	ASP	947	8.300	27.430	0.671	1.00	51.33	6
ATOM	932	CG	ASP	947	6.870	27.122	1.021	1.00	51.33	6
ATOM	933	OD1	ASP	947	6.378	26.066	0.572	1.00	51.33	8
ATOM	934	OD2	ASP	947	6.248	27.934	1.740	1.00	51.33	8
ATOM	935	C	ASP	947	10.231	26.909	-0.772	1.00	24.26	6
ATOM	936	O	ASP	947	10.378	27.109	-1.979	1.00	24.26	8
ATOM	937	N	VAL	948	11.192	27.120	0.123	1.00	17.83	7
ATOM	938	CA	VAL	948	12.458	27.641	-0.335	1.00	17.83	6
ATOM	939	CB	VAL	948	13.483	27.833	0.788	1.00	5.04	6
ATOM	940	CG1	VAL	948	14.786	28.296	0.175	1.00	5.04	6
ATOM	941	CG2	VAL	948	13.012	28.856	1.801	1.00	5.04	6
ATOM	942	C	VAL	948	13.078	26.766	-1.412	1.00	17.83	6
ATOM	943	O	VAL	948	13.514	27.304	-2.425	1.00	17.83	8
ATOM	944	N	ALA	949	13.115	25.442	-1.219	1.00	24.98	7
ATOM	945	CA	ALA	949	13.697	24.531	-2.221	1.00	24.98	6
ATOM	946	CB	ALA	949	13.827	23.129	-1.666	1.00	53.47	6
ATOM	947	C	ALA	949	12.882	24.505	-3.505	1.00	24.98	6
ATOM	948	O	ALA	949	13.440	24.313	-4.576	1.00	24.98	8
ATOM	949	N	ARG	950	11.570	24.716	-3.413	1.00	23.96	7
ATOM	950	CA	ARG	950	10.742	24.733	-4.617	1.00	23.96	6
ATOM	951	CB	ARG	950	9.239	24.736	-4.282	1.00	30.38	6
ATOM	952	CG	ARG	950	8.302	24.244	-5.419	1.00	30.38	6
ATOM	953	CD	ARG	950	6.829	24.454	-5.081	1.00	30.38	6
ATOM	954	NE	ARG	950	6.567	24.306	-3.648	1.00	30.38	7
ATOM	955	CZ	ARG	950	6.313	23.154	-3.030	1.00	30.38	6
ATOM	956	NH1	ARG	950	6.270	22.013	-3.723	1.00	30.38	7
ATOM	957	NH2	ARG	950	6.132	23.146	-1.708	1.00	30.38	7
ATOM	958	C	ARG	950	11.091	25.997	-5.391	1.00	23.96	6

FIG. 3Q

ATOM	959	O	ARG	950	11.089	26.003	-6.617	1.00	23.96	8
ATOM	960	N	GLY	951	11.409	27.064	-4.667	1.00	35.74	7
ATOM	961	CA	GLY	951	11.749	28.315	-5.323	1.00	35.74	6
ATOM	962	C	GLY	951	13.156	28.338	-5.890	1.00	35.74	6
ATOM	963	O	GLY	951	13.439	29.046	-6.850	1.00	35.74	8
ATOM	964	N	MET	952	14.050	27.562	-5.294	1.00	35.49	7
ATOM	965	CA	MET	952	15.430	27.512	-5.755	1.00	35.49	6
ATOM	966	CB	MET	952	16.335	26.979	-4.656	1.00	28.83	6
ATOM	967	CG	MET	952	16.616	27.981	-3.562	1.00	28.83	6
ATOM	968	SD	MET	952	17.396	29.511	-4.180	1.00	28.83	16
ATOM	969	CE	MET	952	18.963	28.883	-4.732	1.00	28.83	6
ATOM	970	C	MET	952	15.553	26.645	-6.972	1.00	35.49	6
ATOM	971	O	MET	952	16.480	26.786	-7.759	1.00	35.49	8
ATOM	972	N	ASP	953	14.623	25.723	-7.119	1.00	22.04	7
ATOM	973	CA	ASP	953	14.658	24.863	-8.277	1.00	22.04	6
ATOM	974	CB	ASP	953	13.701	23.708	-8.065	1.00	46.74	6
ATOM	975	CG	ASP	953	13.868	22.649	-9.095	1.00	46.74	6
ATOM	976	OD1	ASP	953	14.938	22.016	-9.119	1.00	46.74	8
ATOM	977	OD2	ASP	953	12.934	22.479	-9.894	1.00	46.74	8
ATOM	978	C	ASP	953	14.285	25.650	-9.534	1.00	22.04	6
ATOM	979	O	ASP	953	14.796	25.378	-10.600	1.00	22.04	8
ATOM	980	N	TYR	954	13.388	26.620	-9.391	1.00	30.73	7
ATOM	981	CA	TYR	954	12.969	27.454	-10.506	1.00	30.73	6
ATOM	982	CB	TYR	954	11.735	28.261	-10.120	1.00	46.88	6
ATOM	983	CG	TYR	954	11.212	29.222	-11.180	1.00	46.88	6
ATOM	984	CD1	TYR	954	10.358	28.777	-12.198	1.00	46.88	6
ATOM	985	CE1	TYR	954	9.817	29.675	-13.139	1.00	46.88	6
ATOM	986	CD2	TYR	954	11.523	30.596	-11.131	1.00	46.88	6
ATOM	987	CE2	TYR	954	10.987	31.498	-12.071	1.00	46.88	6
ATOM	988	CZ	TYR	954	10.139	31.023	-13.062	1.00	46.88	6
ATOM	989	OH	TYR	954	9.618	31.893	-13.980	1.00	46.88	8
ATOM	990	C	TYR	954	14.104	28.406	-10.820	1.00	30.73	6
ATOM	991	O	TYR	954	14.484	28.556	-11.961	1.00	30.73	8
ATOM	992	N	LEU	955	14.654	29.048	-9.801	1.00	22.51	7
ATOM	993	CA	LEU	955	15.727	29.991	-10.043	1.00	22.51	6
ATOM	994	CB	LEU	955	16.100	30.747	-8.771	1.00	36.85	6
ATOM	995	CG	LEU	955	15.064	31.699	-8.184	1.00	36.85	6
ATOM	996	CD1	LEU	955	15.708	32.365	-7.021	1.00	36.85	6
ATOM	997	CD2	LEU	955	14.586	32.734	-9.210	1.00	36.85	6
ATOM	998	C	LEU	955	16.963	29.355	-10.619	1.00	22.51	6
ATOM	999	O	LEU	955	17.530	29.885	-11.560	1.00	22.51	8
ATOM	1000	N	SER	956	17.403	28.229	-10.080	1.00	31.05	7
ATOM	1001	CA	SER	956	18.608	27.602	-10.615	1.00	31.05	6
ATOM	1002	CB	SER	956	18.998	26.380	-9.778	1.00	57.17	6
ATOM	1003	OG	SER	956	18.077	25.324	-9.989	1.00	57.17	8
ATOM	1004	C	SER	956	18.439	27.207	-12.084	1.00	31.05	6
ATOM	1005	O	SER	956	19.379	27.348	-12.858	1.00	31.05	8
ATOM	1006	N	GLN	957	17.247	26.732	-12.462	1.00	19.64	7
ATOM	1007	CA	GLN	957	16.932	26.307	-13.841	1.00	19.64	6
ATOM	1008	CB	GLN	957	15.580	25.587	-13.899	1.00	97.55	6
ATOM	1009	CG	GLN	957	15.565	24.175	-13.366	1.00	97.55	6
ATOM	1010	CD	GLN	957	16.884	23.460	-13.539	1.00	97.55	6
ATOM	1011	OE1	GLN	957	17.543	23.597	-14.568	1.00	97.55	8
ATOM	1012	NE2	GLN	957	17.275	22.679	-12.532	1.00	97.55	7
ATOM	1013	C	GLN	957	16.901	27.437	-14.860	1.00	19.64	6
ATOM	1014	O	GLN	957	16.903	27.191	-16.054	1.00	19.64	8
ATOM	1015	N	LYS	958	16.815	28.666	-14.370	1.00	37.82	7

FIG. 3R

ATOM	1016	CA	LYS	958	16.801	29.851	-15.205	1.00	37.82	6
ATOM	1017	CB	LYS	958	15.881	30.918	-14.601	1.00	51.85	6
ATOM	1018	CG	LYS	958	14.374	30.580	-14.569	1.00	51.85	6
ATOM	1019	CD	LYS	958	13.831	30.551	-15.986	1.00	51.85	6
ATOM	1020	CE	LYS	958	12.345	30.408	-16.083	1.00	51.85	6
ATOM	1021	NZ	LYS	958	12.076	30.168	-17.526	1.00	51.85	7
ATOM	1022	C	LYS	958	18.236	30.355	-15.192	1.00	37.82	6
ATOM	1023	O	LYS	958	18.528	31.466	-15.641	1.00	37.82	8
ATOM	1024	N	GLN	959	19.129	29.546	-14.634	1.00	37.14	7
ATOM	1025	CA	GLN	959	20.543	29.885	-14.550	1.00	37.14	6
ATOM	1026	CB	GLN	959	21.078	30.229	-15.942	1.00	59.23	6
ATOM	1027	CG	GLN	959	20.943	29.096	-16.925	1.00	59.23	6
ATOM	1028	CD	GLN	959	21.605	27.827	-16.441	1.00	59.23	6
ATOM	1029	OE1	GLN	959	22.832	27.742	-16.372	1.00	59.23	8
ATOM	1030	NE2	GLN	959	20.790	26.844	-16.047	1.00	59.23	7
ATOM	1031	C	GLN	959	20.914	31.004	-13.559	1.00	37.14	6
ATOM	1032	O	GLN	959	21.937	31.669	-13.751	1.00	37.14	8
ATOM	1033	N	PHE	960	20.097	31.201	-12.519	1.00	48.69	7
ATOM	1034	CA	PHE	960	20.369	32.208	-11.492	1.00	48.69	6
ATOM	1035	CB	PHE	960	19.067	32.712	-10.840	1.00	18.22	6
ATOM	1036	CG	PHE	960	18.261	33.647	-11.686	1.00	18.22	6
ATOM	1037	CD1	PHE	960	17.426	33.166	-12.686	1.00	18.22	6
ATOM	1038	CD2	PHE	960	18.343	35.023	-11.493	1.00	18.22	6
ATOM	1039	CE1	PHE	960	16.677	34.044	-13.502	1.00	18.22	6
ATOM	1040	CE2	PHE	960	17.607	35.908	-12.296	1.00	18.22	6
ATOM	1041	CZ	PHE	960	16.777	35.415	-13.301	1.00	18.22	6
ATOM	1042	C	PHE	960	21.225	31.549	-10.402	1.00	48.69	6
ATOM	1043	O	PHE	960	21.203	30.329	-10.251	1.00	48.69	8
ATOM	1044	N	ILE	961	22.000	32.348	-9.674	1.00	25.93	7
ATOM	1045	CA	ILE	961	22.814	31.840	-8.561	1.00	25.93	6
ATOM	1046	CB	ILE	961	24.347	31.827	-8.883	1.00	5.00	6
ATOM	1047	CG2	ILE	961	25.140	31.201	-7.756	1.00	5.00	6
ATOM	1048	CG1	ILE	961	24.610	31.048	-10.132	1.00	5.00	6
ATOM	1049	CD1	ILE	961	25.990	31.281	-10.676	1.00	5.00	6
ATOM	1050	C	ILE	961	22.542	32.864	-7.449	1.00	25.93	6
ATOM	1051	O	ILE	961	22.658	34.061	-7.689	1.00	25.93	8
ATOM	1052	N	HIS	962	22.193	32.412	-6.247	1.00	38.00	7
ATOM	1053	CA	HIS	962	21.871	33.355	-5.180	1.00	38.00	6
ATOM	1054	CB	HIS	962	21.093	32.661	-4.072	1.00	25.73	6
ATOM	1055	CG	HIS	962	20.206	33.579	-3.289	1.00	25.73	6
ATOM	1056	CD2	HIS	962	20.482	34.461	-2.308	1.00	25.73	6
ATOM	1057	ND1	HIS	962	18.846	33.614	-3.475	1.00	25.73	7
ATOM	1058	CE1	HIS	962	18.315	34.478	-2.625	1.00	25.73	6
ATOM	1059	NE2	HIS	962	19.282	35.004	-1.903	1.00	25.73	7
ATOM	1060	C	HIS	962	23.054	34.079	-4.573	1.00	38.00	6
ATOM	1061	O	HIS	962	23.119	35.303	-4.637	1.00	38.00	8
ATOM	1062	N	ARG	963	23.972	33.338	-3.958	1.00	61.33	7
ATOM	1063	CA	ARG	963	25.152	33.932	-3.334	1.00	61.33	6
ATOM	1064	CB	ARG	963	25.855	34.907	-4.306	1.00	42.94	6
ATOM	1065	CG	ARG	963	25.864	34.466	-5.753	1.00	42.94	6
ATOM	1066	CD	ARG	963	26.986	35.078	-6.571	1.00	42.94	6
ATOM	1067	NE	ARG	963	26.799	36.481	-6.929	1.00	42.94	7
ATOM	1068	CZ	ARG	963	26.940	37.488	-6.079	1.00	42.94	6
ATOM	1069	NH1	ARG	963	27.268	37.258	-4.809	1.00	42.94	7
ATOM	1070	NH2	ARG	963	26.752	38.723	-6.508	1.00	42.94	7
ATOM	1071	C	ARG	963	24.756	34.688	-2.062	1.00	61.33	6
ATOM	1072	O	ARG	963	25.543	35.464	-1.528	1.00	61.33	8

FIG. 3S

ATOM	1073	N	ASN	964	23.549	34.460	-1.561	1.00	37.36	7
ATOM	1074	CA	ASN	964	23.111	35.212	-0.384	1.00	37.36	6
ATOM	1075	CB	ASN	964	22.742	36.636	-0.805	1.00	69.75	6
ATOM	1076	CG	ASN	964	23.319	37.670	0.107	1.00	69.75	6
ATOM	1077	OD1	ASN	964	23.337	37.499	1.324	1.00	69.75	8
ATOM	1078	ND2	ASN	964	23.792	38.761	-0.468	1.00	69.75	7
ATOM	1079	C	ASN	964	21.909	34.573	0.273	1.00	37.36	6
ATOM	1080	O	ASN	964	21.096	35.251	0.890	1.00	37.36	8
ATOM	1081	N	LEU	965	21.812	33.258	0.133	1.00	45.72	7
ATOM	1082	CA	LEU	965	20.691	32.503	0.666	1.00	45.72	6
ATOM	1083	CB	LEU	965	20.515	31.230	-0.182	1.00	22.49	6
ATOM	1084	CG	LEU	965	19.348	30.261	-0.002	1.00	22.49	6
ATOM	1085	CD1	LEU	965	19.237	29.344	-1.189	1.00	22.49	6
ATOM	1086	CD2	LEU	965	19.565	29.461	1.252	1.00	22.49	6
ATOM	1087	C	LEU	965	20.867	32.180	2.151	1.00	45.72	6
ATOM	1088	O	LEU	965	21.862	31.584	2.564	1.00	45.72	8
ATOM	1089	N	ALA	966	19.898	32.605	2.948	1.00	9.29	7
ATOM	1090	CA	ALA	966	19.899	32.364	4.386	1.00	9.29	6
ATOM	1091	CB	ALA	966	20.870	33.291	5.057	1.00	5.00	6
ATOM	1092	C	ALA	966	18.474	32.615	4.891	1.00	9.29	6
ATOM	1093	O	ALA	966	17.613	32.963	4.107	1.00	9.29	8
ATOM	1094	N	ALA	967	18.209	32.464	6.181	1.00	20.93	7
ATOM	1095	CA	ALA	967	16.855	32.698	6.627	1.00	20.93	6
ATOM	1096	CB	ALA	967	16.627	32.084	7.989	1.00	8.30	6
ATOM	1097	C	ALA	967	16.481	34.170	6.630	1.00	20.93	6
ATOM	1098	O	ALA	967	15.335	34.486	6.393	1.00	20.93	8
ATOM	1099	N	ARG	968	17.423	35.077	6.875	1.00	18.97	7
ATOM	1100	CA	ARG	968	17.100	36.503	6.901	1.00	18.97	6
ATOM	1101	CB	ARG	968	18.298	37.322	7.381	1.00	55.21	6
ATOM	1102	CG	ARG	968	19.596	36.932	6.747	1.00	55.21	6
ATOM	1103	CD	ARG	968	20.653	38.006	6.946	1.00	55.21	6
ATOM	1104	NE	ARG	968	21.881	37.608	6.275	1.00	55.21	7
ATOM	1105	CZ	ARG	968	22.617	36.572	6.652	1.00	55.21	6
ATOM	1106	NH1	ARG	968	22.246	35.846	7.704	1.00	55.21	7
ATOM	1107	NH2	ARG	968	23.697	36.244	5.954	1.00	55.21	7
ATOM	1108	C	ARG	968	16.632	37.016	5.548	1.00	18.97	6
ATOM	1109	O	ARG	968	15.790	37.915	5.477	1.00	18.97	8
ATOM	1110	N	ASN	969	17.165	36.427	4.481	1.00	17.09	7
ATOM	1111	CA	ASN	969	16.820	36.815	3.109	1.00	17.09	6
ATOM	1112	CB	ASN	969	18.008	36.589	2.179	1.00	47.15	6
ATOM	1113	CG	ASN	969	19.028	37.700	2.240	1.00	47.15	6
ATOM	1114	OD1	ASN	969	20.137	37.547	1.739	1.00	47.15	8
ATOM	1115	ND2	ASN	969	18.661	38.831	2.842	1.00	47.15	7
ATOM	1116	C	ASN	969	15.619	36.088	2.526	1.00	17.09	6
ATOM	1117	O	ASN	969	15.524	35.926	1.318	1.00	17.09	8
ATOM	1118	N	ILE	970	14.725	35.625	3.385	1.00	17.16	7
ATOM	1119	CA	ILE	970	13.527	34.939	2.933	1.00	17.16	6
ATOM	1120	CB	ILE	970	13.521	33.425	3.353	1.00	5.00	6
ATOM	1121	CG2	ILE	970	12.211	32.763	2.943	1.00	5.00	6
ATOM	1122	CG1	ILE	970	14.716	32.686	2.742	1.00	5.00	6
ATOM	1123	CD1	ILE	970	14.542	32.175	1.313	1.00	5.00	6
ATOM	1124	C	ILE	970	12.395	35.687	3.653	1.00	17.16	6
ATOM	1125	O	ILE	970	12.454	35.923	4.864	1.00	17.16	8
ATOM	1126	N	LEU	971	11.365	36.047	2.903	1.00	27.06	7
ATOM	1127	CA	LEU	971	10.234	36.784	3.443	1.00	27.06	6
ATOM	1128	CB	LEU	971	10.000	38.039	2.584	1.00	23.00	6
ATOM	1129	CG	LEU	971	11.152	39.063	2.555	1.00	23.00	6

FIG. 3T

ATOM	1130	CD1	LEU	971	11.197	39.762	1.249	1.00	23.00	6
ATOM	1131	CD2	LEU	971	10.990	40.054	3.689	1.00	23.00	6
ATOM	1132	C	LEU	971	8.984	35.910	3.465	1.00	27.06	6
ATOM	1133	O	LEU	971	8.730	35.192	2.511	1.00	27.06	8
ATOM	1134	N	VAL	972	8.218	35.967	4.558	1.00	35.27	7
ATOM	1135	CA	VAL	972	6.974	35.188	4.710	1.00	35.27	6
ATOM	1136	CB	VAL	972	6.641	34.916	6.237	1.00	15.12	6
ATOM	1137	CG1	VAL	972	5.384	34.069	6.387	1.00	15.12	6
ATOM	1138	CG2	VAL	972	7.806	34.239	6.917	1.00	15.12	6
ATOM	1139	C	VAL	972	5.805	35.979	4.086	1.00	35.27	6
ATOM	1140	O	VAL	972	5.220	36.848	4.727	1.00	35.27	8
ATOM	1141	N	GLY	973	5.466	35.686	2.841	1.00	28.86	7
ATOM	1142	CA	GLY	973	4.378	36.404	2.212	1.00	28.86	6
ATOM	1143	C	GLY	973	3.021	35.983	2.743	1.00	28.86	6
ATOM	1144	O	GLY	973	2.933	35.251	3.734	1.00	28.86	8
ATOM	1145	N	GLU	974	1.954	36.429	2.092	1.00	36.97	7
ATOM	1146	CA	GLU	974	0.621	36.081	2.554	1.00	36.97	6
ATOM	1147	CB	GLU	974	-0.434	36.662	1.619	1.00	98.72	6
ATOM	1148	CG	GLU	974	-1.001	37.980	2.107	1.00	98.72	6
ATOM	1149	CD	GLU	974	-1.619	37.873	3.503	1.00	98.72	6
ATOM	1150	OE1	GLU	974	-2.364	36.904	3.759	1.00	98.72	8
ATOM	1151	OE2	GLU	974	-1.368	38.763	4.342	1.00	98.72	8
ATOM	1152	C	GLU	974	0.418	34.585	2.720	1.00	36.97	6
ATOM	1153	O	GLU	974	1.049	33.768	2.034	1.00	36.97	8
ATOM	1154	N	ASN	975	-0.474	34.253	3.649	1.00	50.17	7
ATOM	1155	CA	ASN	975	-0.811	32.878	3.980	1.00	50.17	6
ATOM	1156	CB	ASN	975	-1.496	32.190	2.812	1.00	49.51	6
ATOM	1157	CG	ASN	975	-2.900	32.725	2.577	1.00	49.51	6
ATOM	1158	OD1	ASN	975	-3.688	32.145	1.834	1.00	49.51	8
ATOM	1159	ND2	ASN	975	-3.218	33.851	3.213	1.00	49.51	7
ATOM	1160	C	ASN	975	0.432	32.122	4.392	1.00	50.17	6
ATOM	1161	O	ASN	975	0.528	30.910	4.222	1.00	50.17	8
ATOM	1162	N	TYR	976	1.386	32.871	4.931	1.00	34.67	7
ATOM	1163	CA	TYR	976	2.637	32.335	5.427	1.00	34.67	6
ATOM	1164	CB	TYR	976	2.386	31.613	6.734	1.00	32.84	6
ATOM	1165	CG	TYR	976	1.690	32.497	7.736	1.00	32.84	6
ATOM	1166	CD1	TYR	976	0.309	32.654	7.715	1.00	32.84	6
ATOM	1167	CE1	TYR	976	-0.328	33.464	8.525	1.00	32.84	6
ATOM	1168	CD2	TYR	976	2.411	33.182	8.693	1.00	32.84	6
ATOM	1169	CE2	TYR	976	1.792	33.991	9.602	1.00	32.84	6
ATOM	1170	CZ	TYR	976	0.422	34.129	9.571	1.00	32.84	6
ATOM	1171	OH	TYR	976	-0.210	34.897	10.515	1.00	32.84	8
ATOM	1172	C	TYR	976	3.376	31.440	4.475	1.00	34.67	6
ATOM	1173	O	TYR	976	3.903	30.410	4.875	1.00	34.67	8
ATOM	1174	N	VAL	977	3.436	31.857	3.217	1.00	16.20	7
ATOM	1175	CA	VAL	977	4.135	31.111	2.181	1.00	16.20	6
ATOM	1176	CB	VAL	977	3.297	31.091	0.876	1.00	9.07	6
ATOM	1177	CG1	VAL	977	4.187	30.767	-0.331	1.00	9.07	6
ATOM	1178	CG2	VAL	977	2.153	30.102	1.005	1.00	9.07	6
ATOM	1179	C	VAL	977	5.490	31.755	1.900	1.00	16.20	6
ATOM	1180	O	VAL	977	5.545	32.795	1.284	1.00	16.20	8
ATOM	1181	N	ALA	978	6.571	31.126	2.337	1.00	15.88	7
ATOM	1182	CA	ALA	978	7.924	31.643	2.141	1.00	15.88	6
ATOM	1183	CB	ALA	978	8.940	30.547	2.489	1.00	21.88	6
ATOM	1184	C	ALA	978	8.238	32.215	0.757	1.00	15.88	6
ATOM	1185	O	ALA	978	7.905	31.630	-0.268	1.00	15.88	8
ATOM	1186	N	LYS	979	8.920	33.352	0.736	1.00	28.57	7

FIG. 3U

ATOM	1187	CA	LYS	979	9.284	34.011	-0.508	1.00	28.57	6
ATOM	1188	CB	LYS	979	8.468	35.289	-0.621	1.00	15.51	6
ATOM	1189	CG	LYS	979	6.969	35.078	-0.838	1.00	15.51	6
ATOM	1190	CD	LYS	979	6.698	34.786	-2.297	1.00	15.51	6
ATOM	1191	CE	LYS	979	5.254	35.044	-2.662	1.00	15.51	6
ATOM	1192	NZ	LYS	979	4.388	34.606	-1.545	1.00	15.51	7
ATOM	1193	C	LYS	979	10.800	34.294	-0.506	1.00	28.57	6
ATOM	1194	O	LYS	979	11.348	34.679	0.525	1.00	28.57	8
ATOM	1195	N	ILE	980	11.458	34.082	-1.655	1.00	23.28	7
ATOM	1196	CA	ILE	980	12.914	34.271	-1.815	1.00	23.28	6
ATOM	1197	CB	ILE	980	13.507	33.236	-2.812	1.00	12.16	6
ATOM	1198	CG2	ILE	980	14.986	33.535	-3.046	1.00	12.16	6
ATOM	1199	CG1	ILE	980	13.309	31.804	-2.268	1.00	12.16	6
ATOM	1200	CD1	ILE	980	13.475	30.688	-3.319	1.00	12.16	6
ATOM	1201	C	ILE	980	13.270	35.665	-2.301	1.00	23.28	6
ATOM	1202	O	ILE	980	12.739	36.135	-3.292	1.00	23.28	8
ATOM	1203	N	ALA	981	14.185	36.335	-1.623	1.00	30.98	7
ATOM	1204	CA	ALA	981	14.538	37.683	-2.040	1.00	30.98	6
ATOM	1205	CB	ALA	981	13.810	38.664	-1.156	1.00	12.02	6
ATOM	1206	C	ALA	981	16.047	37.959	-2.021	1.00	30.98	6
ATOM	1207	O	ALA	981	16.840	37.172	-1.499	1.00	30.98	8
ATOM	1208	N	ASP	982	16.433	39.094	-2.589	1.00	70.73	7
ATOM	1209	CA	ASP	982	17.834	39.511	-2.652	1.00	70.73	6
ATOM	1210	CB	ASP	982	18.327	39.939	-1.272	1.00	99.58	6
ATOM	1211	CG	ASP	982	19.512	40.861	-1.358	1.00	99.58	6
ATOM	1212	OD1	ASP	982	19.287	42.012	-1.783	1.00	99.58	8
ATOM	1213	OD2	ASP	982	20.646	40.436	-1.039	1.00	99.58	8
ATOM	1214	C	ASP	982	18.821	38.488	-3.199	1.00	70.73	6
ATOM	1215	O	ASP	982	19.686	38.005	-2.477	1.00	70.73	8
ATOM	1216	N	PHE	983	18.703	38.184	-4.479	1.00	67.82	7
ATOM	1217	CA	PHE	983	19.595	37.229	-5.095	1.00	67.82	6
ATOM	1218	CB	PHE	983	18.781	36.124	-5.784	1.00	46.69	6
ATOM	1219	CG	PHE	983	17.480	36.593	-6.382	1.00	46.69	6
ATOM	1220	CD1	PHE	983	17.423	37.752	-7.143	1.00	46.69	6
ATOM	1221	CD2	PHE	983	16.317	35.852	-6.222	1.00	46.69	6
ATOM	1222	CE1	PHE	983	16.229	38.166	-7.737	1.00	46.69	6
ATOM	1223	CE2	PHE	983	15.122	36.259	-6.814	1.00	46.69	6
ATOM	1224	CZ	PHE	983	15.080	37.413	-7.570	1.00	46.69	6
ATOM	1225	C	PHE	983	20.552	37.905	-6.081	1.00	67.82	6
ATOM	1226	O	PHE	983	20.451	39.112	-6.338	1.00	67.82	8
ATOM	1227	N	GLY	984	21.497	37.128	-6.599	1.00	44.02	7
ATOM	1228	CA	GLY	984	22.467	37.644	-7.543	1.00	44.02	6
ATOM	1229	C	GLY	984	21.911	37.639	-8.954	1.00	44.02	6
ATOM	1230	O	GLY	984	21.520	36.599	-9.488	1.00	44.02	8
ATOM	1231	N	LEU	985	21.875	38.816	-9.562	1.00	100.00	7
ATOM	1232	CA	LEU	985	21.363	38.951	-10.917	1.00	100.00	6
ATOM	1233	CB	LEU	985	20.792	40.360	-11.126	1.00	41.04	6
ATOM	1234	CG	LEU	985	19.455	40.644	-10.434	1.00	41.04	6
ATOM	1235	CD1	LEU	985	18.448	39.621	-10.945	1.00	41.04	6
ATOM	1236	CD2	LEU	985	19.577	40.549	-8.925	1.00	41.04	6
ATOM	1237	C	LEU	985	22.473	38.670	-11.920	1.00	100.00	6
ATOM	1238	O	LEU	985	22.517	39.253	-13.004	1.00	100.00	8
ATOM	1239	N	SER	986	23.383	37.785	-11.539	1.00	42.70	7
ATOM	1240	CA	SER	986	24.484	37.421	-12.416	1.00	42.70	6
ATOM	1241	CB	SER	986	25.818	37.625	-11.697	1.00	68.70	6
ATOM	1242	OG	SER	986	25.996	38.984	-11.346	1.00	68.70	8
ATOM	1243	C	SER	986	24.295	35.955	-12.780	1.00	42.70	6

FIG. 3V

ATOM	1244	O	SER	986	24.956	35.078	-12.238	1.00	42.70	8
ATOM	1245	N	ARG	987	23.381	35.697	-13.703	1.00	47.12	7
ATOM	1246	CA	ARG	987	23.068	34.336	-14.124	1.00	47.12	6
ATOM	1247	CB	ARG	987	21.873	34.383	-15.045	1.00	55.43	6
ATOM	1248	CG	ARG	987	20.828	35.354	-14.585	1.00	55.43	6
ATOM	1249	CD	ARG	987	19.927	35.581	-15.728	1.00	55.43	6
ATOM	1250	NE	ARG	987	19.371	34.311	-16.169	1.00	55.43	7
ATOM	1251	CZ	ARG	987	18.891	34.116	-17.385	1.00	55.43	6
ATOM	1252	NH1	ARG	987	18.924	35.110	-18.261	1.00	55.43	7
ATOM	1253	NH2	ARG	987	18.364	32.946	-17.713	1.00	55.43	7
ATOM	1254	C	ARG	987	24.204	33.608	-14.823	1.00	47.12	6
ATOM	1255	O	ARG	987	24.990	34.223	-15.535	1.00	47.12	8
ATOM	1256	N	GLY	988	24.281	32.294	-14.629	1.00	32.39	7
ATOM	1257	CA	GLY	988	25.330	31.512	-15.274	1.00	32.39	6
ATOM	1258	C	GLY	988	25.704	30.203	-14.592	1.00	32.39	6
ATOM	1259	O	GLY	988	24.832	29.393	-14.275	1.00	32.39	8
ATOM	1260	N	GLN	989	26.999	29.978	-14.382	1.00	53.32	7
ATOM	1261	CA	GLN	989	27.473	28.756	-13.738	1.00	53.32	6
ATOM	1262	CB	GLN	989	28.063	27.789	-14.761	1.00	52.63	6
ATOM	1263	CG	GLN	989	27.056	26.759	-15.207	1.00	52.63	6
ATOM	1264	CD	GLN	989	27.583	25.337	-15.120	1.00	52.63	6
ATOM	1265	OE1	GLN	989	28.219	24.855	-16.052	1.00	52.63	8
ATOM	1266	NE2	GLN	989	27.355	24.672	-13.985	1.00	52.63	7
ATOM	1267	C	GLN	989	28.473	28.926	-12.631	1.00	53.32	6
ATOM	1268	O	GLN	989	28.683	28.002	-11.861	1.00	53.32	8
ATOM	1269	N	GLU	990	29.082	30.096	-12.532	1.00	57.00	7
ATOM	1270	CA	GLU	990	30.072	30.328	-11.503	1.00	57.00	6
ATOM	1271	CB	GLU	990	31.320	29.532	-11.858	1.00	60.46	6
ATOM	1272	CG	GLU	990	32.281	29.295	-10.745	1.00	60.46	6
ATOM	1273	CD	GLU	990	32.976	27.979	-10.927	1.00	60.46	6
ATOM	1274	OE1	GLU	990	33.448	27.718	-12.049	1.00	60.46	8
ATOM	1275	OE2	GLU	990	33.044	27.198	-9.960	1.00	60.46	8
ATOM	1276	C	GLU	990	30.368	31.814	-11.523	1.00	57.00	6
ATOM	1277	O	GLU	990	30.639	32.363	-12.589	1.00	57.00	8
ATOM	1278	N	VAL	991	30.269	32.470	-10.367	1.00	47.34	7
ATOM	1279	CA	VAL	991	30.567	33.904	-10.285	1.00	47.34	6
ATOM	1280	CB	VAL	991	29.423	34.745	-9.575	1.00	25.98	6
ATOM	1281	CG1	VAL	991	29.646	36.247	-9.822	1.00	25.98	6
ATOM	1282	CG2	VAL	991	28.029	34.365	-10.094	1.00	25.98	6
ATOM	1283	C	VAL	991	31.878	34.057	-9.493	1.00	47.34	6
ATOM	1284	O	VAL	991	32.387	33.090	-8.924	1.00	47.34	8
ATOM	1285	N	TYR	992	32.437	35.262	-9.483	1.00	68.84	7
ATOM	1286	CA	TYR	992	33.683	35.517	-8.774	1.00	68.84	6
ATOM	1287	CB	TYR	992	34.849	35.554	-9.765	1.00	49.61	6
ATOM	1288	CG	TYR	992	36.187	35.817	-9.103	1.00	49.61	6
ATOM	1289	CD1	TYR	992	36.680	34.950	-8.127	1.00	49.61	6
ATOM	1290	CE1	TYR	992	37.886	35.201	-7.465	1.00	49.61	6
ATOM	1291	CD2	TYR	992	36.941	36.947	-9.410	1.00	49.61	6
ATOM	1292	CE2	TYR	992	38.154	37.210	-8.750	1.00	49.61	6
ATOM	1293	CZ	TYR	992	38.614	36.333	-7.780	1.00	49.61	6
ATOM	1294	OH	TYR	992	39.785	36.607	-7.115	1.00	49.61	8
ATOM	1295	C	TYR	992	33.653	36.836	-7.999	1.00	68.84	6
ATOM	1296	O	TYR	992	33.941	37.886	-8.565	1.00	68.84	8
ATOM	1297	N	VAL	993	33.312	36.802	-6.718	1.00	73.45	7
ATOM	1298	CA	VAL	993	33.293	38.048	-5.964	1.00	73.45	6
ATOM	1299	CB	VAL	993	32.078	38.110	-5.043	1.00	77.88	6
ATOM	1300	CG1	VAL	993	30.812	38.281	-5.857	1.00	77.88	6

FIG. 3W.

ATOM	1301	CG2	VAL	993	32.012	36.866	-4.236	1.00	77.88	6
ATOM	1302	C	VAL	993	34.585	38.227	-5.162	1.00	73.45	6
ATOM	1303	O	VAL	993	35.222	37.248	-4.762	1.00	73.45	8
ATOM	1304	N	LYS	994	34.965	39.483	-4.946	1.00	100.00	7
ATOM	1305	CA	LYS	994	36.190	39.825	-4.225	1.00	100.00	6
ATOM	1306	CB	LYS	994	37.340	39.934	-5.227	1.00	96.49	6
ATOM	1307	CG	LYS	994	38.693	40.258	-4.635	1.00	96.49	6
ATOM	1308	CD	LYS	994	39.679	40.656	-5.728	1.00	96.49	6
ATOM	1309	CE	LYS	994	40.977	39.891	-5.576	1.00	96.49	6
ATOM	1310	NZ	LYS	994	41.937	40.208	-6.655	1.00	96.49	7
ATOM	1311	C	LYS	994	35.981	41.170	-3.525	1.00	100.00	6
ATOM	1312	O	LYS	994	36.298	42.217	-4.089	1.00	100.00	8
ATOM	1313	N	LYS	995	35.456	41.135	-2.299	1.00	100.00	7
ATOM	1314	CA	LYS	995	35.173	42.337	-1.505	1.00	100.00	6
ATOM	1315	CB	LYS	995	36.432	43.233	-1.423	1.00	100.00	6
ATOM	1316	C	LYS	995	33.996	43.132	-2.094	1.00	100.00	6
ATOM	1317	O	LYS	995	34.079	44.383	-2.139	1.00	100.00	8
ATOM	1318	OXT	LYS	995	33.001	42.485	-2.484	1.00	85.30	8
TER										
ATOM	1319	CB	PRO	1001	26.968	35.804	4.979	1.00	23.69	6
ATOM	1320	CG	PRO	1001	26.527	36.525	3.738	1.00	23.69	6
ATOM	1321	C	PRO	1001	29.219	34.895	5.215	1.00	43.97	6
ATOM	1322	O	PRO	1001	28.910	33.885	4.598	1.00	43.97	8
ATOM	1323	N	PRO	1001	28.835	36.609	3.692	1.00	43.97	7
ATOM	1324	CD	PRO	1001	27.692	36.488	2.779	1.00	23.69	6
ATOM	1325	CA	PRO	1001	28.434	36.157	5.028	1.00	43.97	6
ATOM	1326	N	VAL	1002	30.217	34.937	6.077	1.00	30.46	7
ATOM	1327	CA	VAL	1002	31.040	33.763	6.267	1.00	30.46	6
ATOM	1328	CB	VAL	1002	32.241	34.137	7.118	1.00	49.80	6
ATOM	1329	CG1	VAL	1002	32.805	35.456	6.632	1.00	49.80	6
ATOM	1330	CG2	VAL	1002	31.852	34.219	8.578	1.00	49.80	6
ATOM	1331	C	VAL	1002	30.360	32.503	6.834	1.00	30.46	6
ATOM	1332	O	VAL	1002	30.790	31.389	6.553	1.00	30.46	8
ATOM	1333	N	ARG	1003	29.292	32.669	7.596	1.00	40.35	7
ATOM	1334	CA	ARG	1003	28.643	31.505	8.207	1.00	40.35	6
ATOM	1335	CB	ARG	1003	27.872	31.924	9.444	1.00	42.33	6
ATOM	1336	CG	ARG	1003	28.755	32.265	10.626	1.00	42.33	6
ATOM	1337	CD	ARG	1003	27.857	32.633	11.767	1.00	42.33	6
ATOM	1338	NE	ARG	1003	28.533	32.694	13.047	1.00	42.33	7
ATOM	1339	CZ	ARG	1003	29.508	33.544	13.336	1.00	42.33	6
ATOM	1340	NH1	ARG	1003	29.932	34.417	12.428	1.00	42.33	7
ATOM	1341	NH2	ARG	1003	30.067	33.516	14.535	1.00	42.33	7
ATOM	1342	C	ARG	1003	27.737	30.626	7.370	1.00	40.35	6
ATOM	1343	O	ARG	1003	27.262	29.606	7.865	1.00	40.35	8
ATOM	1344	N	TRP	1004	27.495	31.011	6.121	1.00	26.04	7
ATOM	1345	CA	TRP	1004	26.632	30.250	5.221	1.00	26.04	6
ATOM	1346	CB	TRP	1004	25.459	31.141	4.768	1.00	50.68	6
ATOM	1347	CG	TRP	1004	24.332	31.279	5.776	1.00	50.68	6
ATOM	1348	CD2	TRP	1004	24.261	32.186	6.885	1.00	50.68	6
ATOM	1349	CE2	TRP	1004	23.066	31.901	7.585	1.00	50.68	6
ATOM	1350	CE3	TRP	1004	25.093	33.208	7.363	1.00	50.68	6
ATOM	1351	CD1	TRP	1004	23.207	30.513	5.843	1.00	50.68	6
ATOM	1352	NE1	TRP	1004	22.445	30.880	6.924	1.00	50.68	7
ATOM	1353	CZ2	TRP	1004	22.681	32.601	8.737	1.00	50.68	6
ATOM	1354	CZ3	TRP	1004	24.704	33.905	8.515	1.00	50.68	6
ATOM	1355	CH2	TRP	1004	23.510	33.594	9.186	1.00	50.68	6
ATOM	1356	C	TRP	1004	27.409	29.747	4.006	1.00	26.04	6

FIG. 3X

ATOM	1357	O	TRP	1004	27.003	28.794	3.356	1.00	26.04	8
ATOM	1358	N	MET	1005	28.535	30.382	3.706	1.00	37.80	7
ATOM	1359	CA	MET	1005	29.329	30.009	2.543	1.00	37.80	6
ATOM	1360	CB	MET	1005	30.502	30.949	2.412	1.00	40.16	6
ATOM	1361	CG	MET	1005	30.063	32.299	1.973	1.00	40.16	6
ATOM	1362	SD	MET	1005	31.319	33.493	2.212	1.00	40.16	16
ATOM	1363	CE	MET	1005	32.621	32.780	1.246	1.00	40.16	6
ATOM	1364	C	MET	1005	29.827	28.584	2.473	1.00	37.80	6
ATOM	1365	O	MET	1005	30.268	28.011	3.465	1.00	37.80	8
ATOM	1366	N	ALA	1006	29.753	28.008	1.283	1.00	45.98	7
ATOM	1367	CA	ALA	1006	30.230	26.654	1.092	1.00	45.98	6
ATOM	1368	CB	ALA	1006	29.797	26.138	-0.284	1.00	10.86	6
ATOM	1369	C	ALA	1006	31.764	26.736	1.196	1.00	45.98	6
ATOM	1370	O	ALA	1006	32.322	27.830	1.151	1.00	45.98	8
ATOM	1371	N	ILE	1007	32.448	25.604	1.326	1.00	44.58	7
ATOM	1372	CA	ILE	1007	33.909	25.657	1.446	1.00	44.58	6
ATOM	1373	CB	ILE	1007	34.528	24.267	1.753	1.00	25.13	6
ATOM	1374	CG2	ILE	1007	34.415	23.969	3.224	1.00	25.13	6
ATOM	1375	CG1	ILE	1007	33.880	23.182	0.886	1.00	25.13	6
ATOM	1376	CD1	ILE	1007	34.418	23.123	-0.571	1.00	25.13	6
ATOM	1377	C	ILE	1007	34.619	26.244	0.234	1.00	44.58	6
ATOM	1378	O	ILE	1007	35.585	26.988	0.379	1.00	44.58	8
ATOM	1379	N	GLU	1008	34.137	25.915	-0.957	1.00	31.07	7
ATOM	1380	CA	GLU	1008	34.743	26.402	-2.188	1.00	31.07	6
ATOM	1381	CB	GLU	1008	34.089	25.710	-3.378	1.00	43.81	6
ATOM	1382	CG	GLU	1008	32.595	25.941	-3.415	1.00	43.81	6
ATOM	1383	CD	GLU	1008	31.795	24.661	-3.241	1.00	43.81	6
ATOM	1384	OE1	GLU	1008	31.967	23.953	-2.216	1.00	43.81	8
ATOM	1385	OE2	GLU	1008	30.965	24.377	-4.125	1.00	43.81	8
ATOM	1386	C	GLU	1008	34.578	27.914	-2.308	1.00	31.07	6
ATOM	1387	O	GLU	1008	35.377	28.583	-2.967	1.00	31.07	8
ATOM	1388	N	SER	1009	33.546	28.447	-1.660	1.00	30.15	7
ATOM	1389	CA	SER	1009	33.259	29.873	-1.711	1.00	30.15	6
ATOM	1390	CB	SER	1009	31.802	30.117	-1.366	1.00	23.09	6
ATOM	1391	OG	SER	1009	30.984	29.174	-2.034	1.00	23.09	8
ATOM	1392	C	SER	1009	34.150	30.622	-0.743	1.00	30.15	6
ATOM	1393	O	SER	1009	34.565	31.760	-0.995	1.00	30.15	8
ATOM	1394	N	LEU	1010	34.428	29.977	0.381	1.00	29.90	7
ATOM	1395	CA	LEU	1010	35.293	30.566	1.380	1.00	29.90	6
ATOM	1396	CB	LEU	1010	35.402	29.629	2.585	1.00	44.65	6
ATOM	1397	CG	LEU	1010	34.152	29.450	3.460	1.00	44.65	6
ATOM	1398	CD1	LEU	1010	34.435	28.420	4.534	1.00	44.65	6
ATOM	1399	CD2	LEU	1010	33.752	30.781	4.101	1.00	44.65	6
ATOM	1400	C	LEU	1010	36.663	30.771	0.726	1.00	29.90	6
ATOM	1401	O	LEU	1010	37.082	31.912	0.503	1.00	29.90	8
ATOM	1402	N	ASN	1011	37.327	29.661	0.397	1.00	34.23	7
ATOM	1403	CA	ASN	1011	38.652	29.638	-0.230	1.00	34.23	6
ATOM	1404	CB	ASN	1011	39.105	28.205	-0.511	1.00	32.72	6
ATOM	1405	CG	ASN	1011	38.990	27.287	0.679	1.00	32.72	6
ATOM	1406	OD1	ASN	1011	39.433	27.600	1.783	1.00	32.72	8
ATOM	1407	ND2	ASN	1011	38.404	26.117	0.450	1.00	32.72	7
ATOM	1408	C	ASN	1011	38.801	30.353	-1.560	1.00	34.23	6
ATOM	1409	O	ASN	1011	39.728	31.137	-1.748	1.00	34.23	8
ATOM	1410	N	TYR	1012	37.914	30.041	-2.494	1.00	35.06	7
ATOM	1411	CA	TYR	1012	38.018	30.611	-3.822	1.00	35.06	6
ATOM	1412	CB	TYR	1012	37.824	29.521	-4.845	1.00	40.77	6
ATOM	1413	CG	TYR	1012	38.705	28.358	-4.552	1.00	40.77	6

FIG. 3Y

ATOM	1414	CD1	TYR	1012	38.167	27.093	-4.400	1.00	40.77	6
ATOM	1415	CE1	TYR	1012	38.961	26.024	-4.105	1.00	40.77	6
ATOM	1416	CD2	TYR	1012	40.077	28.531	-4.397	1.00	40.77	6
ATOM	1417	CE2	TYR	1012	40.896	27.472	-4.098	1.00	40.77	6
ATOM	1418	CZ	TYR	1012	40.336	26.208	-3.957	1.00	40.77	6
ATOM	1419	OH	TYR	1012	41.152	25.119	-3.717	1.00	40.77	8
ATOM	1420	C	TYR	1012	37.161	31.787	-4.193	1.00	35.06	6
ATOM	1421	O	TYR	1012	37.443	32.440	-5.195	1.00	35.06	8
ATOM	1422	N	SER	1013	36.109	32.060	-3.433	1.00	42.36	7
ATOM	1423	CA	SER	1013	35.278	33.209	-3.746	1.00	42.36	6
ATOM	1424	CB	SER	1013	36.159	34.439	-3.983	1.00	39.37	6
ATOM	1425	OG	SER	1013	37.157	34.576	-2.983	1.00	39.37	8
ATOM	1426	C	SER	1013	34.433	32.973	-4.982	1.00	42.36	6
ATOM	1427	O	SER	1013	34.291	33.865	-5.807	1.00	42.36	8
ATOM	1428	N	VAL	1014	33.890	31.772	-5.121	1.00	22.55	7
ATOM	1429	CA	VAL	1014	33.045	31.467	-6.260	1.00	22.55	6
ATOM	1430	CB	VAL	1014	33.653	30.369	-7.143	1.00	31.51	6
ATOM	1431	CG1	VAL	1014	35.048	30.791	-7.599	1.00	31.51	6
ATOM	1432	CG2	VAL	1014	33.701	29.054	-6.383	1.00	31.51	6
ATOM	1433	C	VAL	1014	31.720	30.999	-5.712	1.00	22.55	6
ATOM	1434	O	VAL	1014	31.644	30.562	-4.577	1.00	22.55	8
ATOM	1435	N	TYR	1015	30.671	31.121	-6.507	1.00	26.01	7
ATOM	1436	CA	TYR	1015	29.338	30.712	-6.101	1.00	26.01	6
ATOM	1437	CB	TYR	1015	28.501	31.938	-5.753	1.00	41.40	6
ATOM	1438	CG	TYR	1015	29.116	32.782	-4.672	1.00	41.40	6
ATOM	1439	CD1	TYR	1015	30.233	33.560	-4.922	1.00	41.40	6
ATOM	1440	CE1	TYR	1015	30.854	34.235	-3.904	1.00	41.40	6
ATOM	1441	CD2	TYR	1015	28.638	32.709	-3.365	1.00	41.40	6
ATOM	1442	CE2	TYR	1015	29.257	33.388	-2.330	1.00	41.40	6
ATOM	1443	CZ	TYR	1015	30.361	34.139	-2.605	1.00	41.40	6
ATOM	1444	OH	TYR	1015	30.968	34.830	-1.588	1.00	41.40	8
ATOM	1445	C	TYR	1015	28.674	29.998	-7.252	1.00	26.01	6
ATOM	1446	O	TYR	1015	28.513	30.572	-8.324	1.00	26.01	8
ATOM	1447	N	THR	1016	28.311	28.741	-7.043	1.00	17.46	7
ATOM	1448	CA	THR	1016	27.610	27.971	-8.082	1.00	17.46	6
ATOM	1449	CB	THR	1016	28.317	26.625	-8.456	1.00	15.11	6
ATOM	1450	OG1	THR	1016	28.649	25.909	-7.262	1.00	15.11	8
ATOM	1451	CG2	THR	1016	29.540	26.855	-9.283	1.00	15.11	6
ATOM	1452	C	THR	1016	26.257	27.590	-7.487	1.00	17.46	6
ATOM	1453	O	THR	1016	25.919	28.038	-6.408	1.00	17.46	8
ATOM	1454	N	THR	1017	25.489	26.752	-8.171	1.00	10.55	7
ATOM	1455	CA	THR	1017	24.229	26.325	-7.585	1.00	10.55	6
ATOM	1456	CB	THR	1017	23.346	25.602	-8.600	1.00	29.18	6
ATOM	1457	OG1	THR	1017	22.913	26.533	-9.600	1.00	29.18	8
ATOM	1458	CG2	THR	1017	22.138	25.017	-7.906	1.00	29.18	6
ATOM	1459	C	THR	1017	24.563	25.381	-6.419	1.00	10.55	6
ATOM	1460	O	THR	1017	23.802	25.287	-5.466	1.00	10.55	8
ATOM	1461	N	ASN	1018	25.740	24.743	-6.500	1.00	41.35	7
ATOM	1462	CA	ASN	1018	26.266	23.772	-5.505	1.00	41.35	6
ATOM	1463	CB	ASN	1018	27.522	23.095	-6.033	1.00	49.00	6
ATOM	1464	CG	ASN	1018	27.234	22.010	-7.015	1.00	49.00	6
ATOM	1465	OD1	ASN	1018	28.100	21.630	-7.788	1.00	49.00	8
ATOM	1466	ND2	ASN	1018	26.025	21.477	-6.981	1.00	49.00	7
ATOM	1467	C	ASN	1018	26.646	24.371	-4.156	1.00	41.35	6
ATOM	1468	O	ASN	1018	26.773	23.647	-3.160	1.00	41.35	8
ATOM	1469	N	SER	1019	26.887	25.680	-4.148	1.00	46.21	7
ATOM	1470	CA	SER	1019	27.247	26.400	-2.935	1.00	46.21	6

FIG. 3Z

ATOM	1471	CB	SER	1019	28.179	27.570	-3.247	1.00	35.31	6
ATOM	1472	OG	SER	1019	27.517	28.561	-3.996	1.00	35.31	8
ATOM	1473	C	SER	1019	25.936	26.919	-2.392	1.00	46.21	6
ATOM	1474	O	SER	1019	25.835	27.281	-1.225	1.00	46.21	8
ATOM	1475	N	ASP	1020	24.929	26.965	-3.253	1.00	42.68	7
ATOM	1476	CA	ASP	1020	23.640	27.426	-2.808	1.00	42.68	6
ATOM	1477	CB	ASP	1020	22.826	28.008	-3.951	1.00	34.86	6
ATOM	1478	CG	ASP	1020	22.962	29.508	-4.032	1.00	34.86	6
ATOM	1479	OD1	ASP	1020	23.242	30.127	-2.972	1.00	34.86	8
ATOM	1480	OD2	ASP	1020	22.788	30.046	-5.149	1.00	34.86	8
ATOM	1481	C	ASP	1020	22.912	26.281	-2.171	1.00	42.68	6
ATOM	1482	O	ASP	1020	21.925	26.487	-1.480	1.00	42.68	8
ATOM	1483	N	VAL	1021	23.401	25.071	-2.398	1.00	33.68	7
ATOM	1484	CA	VAL	1021	22.751	23.944	-1.787	1.00	33.68	6
ATOM	1485	CB	VAL	1021	22.872	22.690	-2.628	1.00	9.47	6
ATOM	1486	CG1	VAL	1021	22.096	21.575	-1.962	1.00	9.47	6
ATOM	1487	CG2	VAL	1021	22.328	22.940	-4.008	1.00	9.47	6
ATOM	1488	C	VAL	1021	23.403	23.746	-0.444	1.00	33.68	6
ATOM	1489	O	VAL	1021	22.872	23.061	0.422	1.00	33.68	8
ATOM	1490	N	TRP	1022	24.565	24.355	-0.268	1.00	49.04	7
ATOM	1491	CA	TRP	1022	25.247	24.284	1.011	1.00	49.04	6
ATOM	1492	CB	TRP	1022	26.732	24.600	0.868	1.00	36.23	6
ATOM	1493	CG	TRP	1022	27.463	24.712	2.164	1.00	36.23	6
ATOM	1494	CD2	TRP	1022	28.575	23.920	2.583	1.00	36.23	6
ATOM	1495	CE2	TRP	1022	28.985	24.411	3.836	1.00	36.23	6
ATOM	1496	CE3	TRP	1022	29.269	22.843	2.019	1.00	36.23	6
ATOM	1497	CD1	TRP	1022	27.246	25.623	3.158	1.00	36.23	6
ATOM	1498	NE1	TRP	1022	28.155	25.452	4.165	1.00	36.23	7
ATOM	1499	CZ2	TRP	1022	30.061	23.862	4.532	1.00	36.23	6
ATOM	1500	CZ3	TRP	1022	30.338	22.300	2.710	1.00	36.23	6
ATOM	1501	CH2	TRP	1022	30.721	22.808	3.951	1.00	36.23	6
ATOM	1502	C	TRP	1022	24.558	25.391	1.777	1.00	49.04	6
ATOM	1503	O	TRP	1022	23.962	25.164	2.822	1.00	49.04	8
ATOM	1504	N	SER	1023	24.599	26.598	1.244	1.00	20.71	7
ATOM	1505	CA	SER	1023	23.946	27.666	1.954	1.00	20.71	6
ATOM	1506	CB	SER	1023	24.032	28.977	1.181	1.00	17.98	6
ATOM	1507	OG	SER	1023	25.377	29.363	1.081	1.00	17.98	8
ATOM	1508	C	SER	1023	22.516	27.305	2.265	1.00	20.71	6
ATOM	1509	O	SER	1023	22.009	27.705	3.298	1.00	20.71	8
ATOM	1510	N	TYR	1024	21.842	26.557	1.400	1.00	27.47	7
ATOM	1511	CA	TYR	1024	20.474	26.200	1.758	1.00	27.47	6
ATOM	1512	CB	TYR	1024	19.728	25.580	0.590	1.00	25.94	6
ATOM	1513	CG	TYR	1024	18.447	24.902	1.003	1.00	25.94	6
ATOM	1514	CD1	TYR	1024	17.222	25.512	0.847	1.00	25.94	6
ATOM	1515	CE1	TYR	1024	16.037	24.846	1.170	1.00	25.94	6
ATOM	1516	CD2	TYR	1024	18.465	23.611	1.506	1.00	25.94	6
ATOM	1517	CE2	TYR	1024	17.288	22.954	1.833	1.00	25.94	6
ATOM	1518	CZ	TYR	1024	16.089	23.579	1.656	1.00	25.94	6
ATOM	1519	OH	TYR	1024	14.949	22.909	1.953	1.00	25.94	8
ATOM	1520	C	TYR	1024	20.502	25.233	2.942	1.00	27.47	6
ATOM	1521	O	TYR	1024	19.712	25.368	3.873	1.00	27.47	8
ATOM	1522	N	GLY	1025	21.419	24.273	2.917	1.00	24.43	7
ATOM	1523	CA	GLY	1025	21.505	23.344	4.025	1.00	24.43	6
ATOM	1524	C	GLY	1025	21.593	24.073	5.356	1.00	24.43	6
ATOM	1525	O	GLY	1025	21.032	23.619	6.356	1.00	24.43	8
ATOM	1526	N	VAL	1026	22.307	25.195	5.384	1.00	31.88	7
ATOM	1527	CA	VAL	1026	22.417	25.947	6.632	1.00	31.88	6

FIG. 3AA

ATOM	1528	CB	VAL	1026	23.566	26.979	6.609	1.00	14.56	6
ATOM	1529	CG1	VAL	1026	23.783	27.551	8.015	1.00	14.56	6
ATOM	1530	CG2	VAL	1026	24.835	26.301	6.132	1.00	14.56	6
ATOM	1531	C	VAL	1026	21.077	26.636	6.908	1.00	31.88	6
ATOM	1532	O	VAL	1026	20.691	26.833	8.062	1.00	31.88	8
ATOM	1533	N	LEU	1027	20.348	26.978	5.855	1.00	36.84	7
ATOM	1534	CA	LEU	1027	19.063	27.591	6.078	1.00	36.84	6
ATOM	1535	CB	LEU	1027	18.470	28.110	4.777	1.00	5.00	6
ATOM	1536	CG	LEU	1027	17.030	28.620	4.806	1.00	5.00	6
ATOM	1537	CD1	LEU	1027	16.683	29.318	6.095	1.00	5.00	6
ATOM	1538	CD2	LEU	1027	16.893	29.549	3.640	1.00	5.00	6
ATOM	1539	C	LEU	1027	18.149	26.556	6.711	1.00	36.84	6
ATOM	1540	O	LEU	1027	17.383	26.885	7.606	1.00	36.84	8
ATOM	1541	N	LEU	1028	18.234	25.304	6.272	1.00	19.77	7
ATOM	1542	CA	LEU	1028	17.390	24.264	6.848	1.00	19.77	6
ATOM	1543	CB	LEU	1028	17.645	22.931	6.147	1.00	24.80	6
ATOM	1544	CG	LEU	1028	16.802	21.696	6.487	1.00	24.80	6
ATOM	1545	CD1	LEU	1028	15.298	21.976	6.507	1.00	24.80	6
ATOM	1546	CD2	LEU	1028	17.117	20.681	5.417	1.00	24.80	6
ATOM	1547	C	LEU	1028	17.681	24.145	8.339	1.00	19.77	6
ATOM	1548	O	LEU	1028	16.779	23.912	9.136	1.00	19.77	8
ATOM	1549	N	TRP	1029	18.944	24.309	8.714	1.00	26.73	7
ATOM	1550	CA	TRP	1029	19.318	24.241	10.114	1.00	26.73	6
ATOM	1551	CB	TRP	1029	20.836	24.229	10.257	1.00	36.84	6
ATOM	1552	CG	TRP	1029	21.363	24.082	11.678	1.00	36.84	6
ATOM	1553	CD2	TRP	1029	21.634	25.145	12.611	1.00	36.84	6
ATOM	1554	CE2	TRP	1029	22.215	24.556	13.757	1.00	36.84	6
ATOM	1555	CE3	TRP	1029	21.438	26.536	12.588	1.00	36.84	6
ATOM	1556	CD1	TRP	1029	21.774	22.926	12.292	1.00	36.84	6
ATOM	1557	NE1	TRP	1029	22.292	23.202	13.539	1.00	36.84	7
ATOM	1558	CZ2	TRP	1029	22.613	25.310	14.860	1.00	36.84	6
ATOM	1559	CZ3	TRP	1029	21.830	27.283	13.682	1.00	36.84	6
ATOM	1560	CH2	TRP	1029	22.409	26.670	14.803	1.00	36.84	6
ATOM	1561	C	TRP	1029	18.736	25.435	10.898	1.00	26.73	6
ATOM	1562	O	TRP	1029	18.498	25.314	12.089	1.00	26.73	8
ATOM	1563	N	GLU	1030	18.520	26.590	10.266	1.00	28.62	7
ATOM	1564	CA	GLU	1030	17.958	27.734	10.996	1.00	28.62	6
ATOM	1565	CB	GLU	1030	18.082	29.020	10.177	1.00	33.13	6
ATOM	1566	CG	GLU	1030	19.486	29.535	10.077	1.00	33.13	6
ATOM	1567	CD	GLU	1030	19.635	30.718	9.135	1.00	33.13	6
ATOM	1568	OE1	GLU	1030	19.628	30.498	7.909	1.00	33.13	8
ATOM	1569	OE2	GLU	1030	19.756	31.865	9.625	1.00	33.13	8
ATOM	1570	C	GLU	1030	16.494	27.467	11.333	1.00	28.62	6
ATOM	1571	O	GLU	1030	16.066	27.619	12.470	1.00	28.62	8
ATOM	1572	N	ILE	1031	15.746	27.065	10.314	1.00	23.86	7
ATOM	1573	CA	ILE	1031	14.328	26.733	10.413	1.00	23.86	6
ATOM	1574	CB	ILE	1031	13.845	26.094	9.083	1.00	5.00	6
ATOM	1575	CG2	ILE	1031	12.626	25.263	9.308	1.00	5.00	6
ATOM	1576	CG1	ILE	1031	13.660	27.181	8.029	1.00	5.00	6
ATOM	1577	CD1	ILE	1031	13.157	26.703	6.709	1.00	5.00	6
ATOM	1578	C	ILE	1031	14.085	25.760	11.544	1.00	23.86	6
ATOM	1579	O	ILE	1031	13.202	25.946	12.357	1.00	23.86	8
ATOM	1580	N	VAL	1032	14.894	24.723	11.595	1.00	16.66	7
ATOM	1581	CA	VAL	1032	14.745	23.717	12.611	1.00	16.66	6
ATOM	1582	CB	VAL	1032	15.538	22.452	12.184	1.00	12.88	6
ATOM	1583	CG1	VAL	1032	15.873	21.594	13.367	1.00	12.88	6
ATOM	1584	CG2	VAL	1032	14.713	21.662	11.163	1.00	12.88	6

FIG. 3BB

ATOM	1585	C	VAL	1032	15.155	24.252	13.977	1.00	16.66	6
ATOM	1586	O	VAL	1032	14.456	24.032	14.952	1.00	16.66	8
ATOM	1587	N	SER	1033	16.258	24.986	14.058	1.00	33.94	7
ATOM	1588	CA	SER	1033	16.732	25.551	15.331	1.00	33.94	6
ATOM	1589	CB	SER	1033	18.173	25.982	15.197	1.00	27.55	6
ATOM	1590	OG	SER	1033	18.203	27.172	14.452	1.00	27.55	8
ATOM	1591	C	SER	1033	15.937	26.791	15.793	1.00	33.94	6
ATOM	1592	O	SER	1033	16.275	27.415	16.801	1.00	33.94	8
ATOM	1593	N	LEU	1034	14.913	27.165	15.035	1.00	25.63	7
ATOM	1594	CA	LEU	1034	14.075	28.313	15.353	1.00	25.63	6
ATOM	1595	CB	LEU	1034	13.382	28.107	16.707	1.00	16.09	6
ATOM	1596	CG	LEU	1034	12.545	26.834	15.882	1.00	16.09	6
ATOM	1597	CD1	LEU	1034	11.931	26.831	18.286	1.00	16.09	6
ATOM	1598	CD2	LEU	1034	11.456	26.758	15.839	1.00	16.09	6
ATOM	1599	C	LEU	1034	14.777	29.676	15.328	1.00	25.63	6
ATOM	1600	O	LEU	1034	14.641	30.476	16.254	1.00	25.63	8
ATOM	1601	N	GLY	1035	15.519	29.927	14.256	1.00	32.06	7
ATOM	1602	CA	GLY	1035	16.185	31.202	14.092	1.00	32.06	6
ATOM	1603	C	GLY	1035	17.458	31.404	14.866	1.00	32.06	6
ATOM	1604	O	GLY	1035	17.832	32.537	15.149	1.00	32.06	8
ATOM	1605	N	GLY	1036	18.124	30.316	15.224	1.00	12.96	7
ATOM	1606	CA	GLY	1036	19.371	30.430	15.957	1.00	12.96	6
ATOM	1607	C	GLY	1036	20.486	30.704	14.974	1.00	12.96	6
ATOM	1608	O	GLY	1036	20.355	30.393	13.789	1.00	12.96	8
ATOM	1609	N	THR	1037	21.572	31.293	15.457	1.00	38.43	7
ATOM	1610	CA	THR	1037	22.712	31.608	14.609	1.00	38.43	6
ATOM	1611	CB	THR	1037	23.593	32.723	15.266	1.00	32.45	6
ATOM	1612	OG1	THR	1037	22.813	33.907	15.442	1.00	32.45	8
ATOM	1613	CG2	THR	1037	24.754	33.076	14.387	1.00	32.45	6
ATOM	1614	C	THR	1037	23.519	30.323	14.418	1.00	38.43	6
ATOM	1615	O	THR	1037	23.687	29.555	15.359	1.00	38.43	8
ATOM	1616	N	PRO	1038	24.003	30.054	13.193	1.00	51.13	7
ATOM	1617	CD	PRO	1038	23.734	30.837	11.973	1.00	42.78	6
ATOM	1618	CA	PRO	1038	24.791	28.859	12.863	1.00	51.13	6
ATOM	1619	CB	PRO	1038	24.677	28.776	11.354	1.00	42.78	6
ATOM	1620	CG	PRO	1038	24.691	30.218	10.977	1.00	42.78	6
ATOM	1621	C	PRO	1038	26.233	28.968	13.308	1.00	51.13	6
ATOM	1622	O	PRO	1038	26.873	30.002	13.113	1.00	51.13	8
ATOM	1623	N	TYR	1039	26.753	27.895	13.886	1.00	44.91	7
ATOM	1624	CA	TYR	1039	28.124	27.909	14.349	1.00	44.91	6
ATOM	1625	CB	TYR	1039	29.082	28.341	13.221	1.00	38.97	6
ATOM	1626	CG	TYR	1039	28.980	27.544	11.933	1.00	38.97	6
ATOM	1627	CD1	TYR	1039	28.593	28.161	10.739	1.00	38.97	6
ATOM	1628	CE1	TYR	1039	28.487	27.434	9.545	1.00	38.97	6
ATOM	1629	CD2	TYR	1039	29.263	26.185	11.907	1.00	38.97	6
ATOM	1630	CE2	TYR	1039	29.165	25.455	10.730	1.00	38.97	6
ATOM	1631	CZ	TYR	1039	28.773	26.082	9.553	1.00	38.97	6
ATOM	1632	OH	TYR	1039	28.647	25.353	8.396	1.00	38.97	8
ATOM	1633	C	TYR	1039	28.176	28.932	15.479	1.00	44.91	6
ATOM	1634	O	TYR	1039	29.152	29.674	15.601	1.00	44.91	8
ATOM	1635	N	CYS	1040	27.120	28.989	16.293	1.00	52.33	7
ATOM	1636	CA	CYS	1040	27.093	29.933	17.411	1.00	52.33	6
ATOM	1637	CB	CYS	1040	25.700	30.015	18.046	1.00	51.31	6
ATOM	1638	SG	CYS	1040	25.484	31.409	19.213	1.00	51.31	16
ATOM	1639	C	CYS	1040	28.094	29.416	18.424	1.00	52.33	6
ATOM	1640	O	CYS	1040	28.113	28.224	18.729	1.00	52.33	8
ATOM	1641	N	GLY	1041	28.930	30.315	18.928	1.00	33.04	7

FIG. 3CC

ATOM	1642	CA	GLY	1041	29.930	29.917	19.895	1.00	33.04	6
ATOM	1643	C	GLY	1041	31.293	29.745	19.257	1.00	33.04	6
ATOM	1644	O	GLY	1041	32.207	29.176	19.855	1.00	33.04	8
ATOM	1645	N	MET	1042	31.435	30.206	18.024	1.00	54.51	7
ATOM	1646	CA	MET	1042	32.718	30.129	17.350	1.00	54.51	6
ATOM	1647	CB	MET	1042	32.703	29.085	16.241	1.00	40.53	6
ATOM	1648	CG	MET	1042	33.032	27.691	16.710	1.00	40.53	6
ATOM	1649	SD	MET	1042	32.920	26.501	15.349	1.00	40.53	16
ATOM	1650	CE	MET	1042	31.539	25.362	15.966	1.00	40.53	6
ATOM	1651	C	MET	1042	33.029	31.492	16.785	1.00	54.51	6
ATOM	1652	O	MET	1042	32.195	32.395	16.804	1.00	54.51	8
ATOM	1653	N	THR	1043	34.241	31.633	16.286	1.00	54.86	7
ATOM	1654	CA	THR	1043	34.677	32.894	15.726	1.00	54.86	6
ATOM	1655	CB	THR	1043	36.055	33.252	16.229	1.00	82.76	6
ATOM	1656	OG1	THR	1043	36.987	32.269	15.763	1.00	82.76	8
ATOM	1657	CG2	THR	1043	36.069	33.282	17.735	1.00	82.76	6
ATOM	1658	C	THR	1043	34.780	32.796	14.227	1.00	54.86	6
ATOM	1659	O	THR	1043	34.695	31.710	13.659	1.00	54.86	8
ATOM	1660	N	CYS	1044	35.002	33.943	13.599	1.00	95.17	7
ATOM	1661	CA	CYS	1044	35.142	34.000	12.158	1.00	95.17	6
ATOM	1662	CB	CYS	1044	35.205	35.453	11.692	1.00	93.17	6
ATOM	1663	SG	CYS	1044	33.676	36.379	11.856	1.00	93.17	16
ATOM	1664	C	CYS	1044	36.396	33.272	11.681	1.00	95.17	6
ATOM	1665	O	CYS	1044	36.622	33.174	10.483	1.00	95.17	8
ATOM	1666	N	ALA	1045	37.215	32.773	12.603	1.00	38.28	7
ATOM	1667	CA	ALA	1045	38.428	32.079	12.197	1.00	38.28	6
ATOM	1668	CB	ALA	1045	39.618	32.633	12.941	1.00	50.33	6
ATOM	1669	C	ALA	1045	38.348	30.571	12.387	1.00	38.28	6
ATOM	1670	O	ALA	1045	38.780	29.817	11.517	1.00	38.28	8
ATOM	1671	N	GLU	1046	37.822	30.131	13.526	1.00	39.84	7
ATOM	1672	CA	GLU	1046	37.712	28.702	13.787	1.00	39.84	6
ATOM	1673	CB	GLU	1046	36.911	28.460	15.068	1.00	83.44	6
ATOM	1674	CG	GLU	1046	37.622	28.995	16.300	1.00	83.44	6
ATOM	1675	CD	GLU	1046	36.997	28.556	17.607	1.00	83.44	6
ATOM	1676	OE1	GLU	1046	36.872	27.334	17.835	1.00	83.44	8
ATOM	1677	OE2	GLU	1046	36.635	29.442	18.408	1.00	83.44	8
ATOM	1678	C	GLU	1046	37.051	28.027	12.591	1.00	39.84	6
ATOM	1679	O	GLU	1046	37.370	26.884	12.245	1.00	39.84	8
ATOM	1680	N	LEU	1047	36.148	28.772	11.953	1.00	55.18	7
ATOM	1681	CA	LEU	1047	35.412	28.312	10.771	1.00	55.18	6
ATOM	1682	CB	LEU	1047	34.315	29.319	10.424	1.00	58.88	6
ATOM	1683	CG	LEU	1047	33.325	29.563	11.565	1.00	58.88	6
ATOM	1684	CD1	LEU	1047	32.333	30.619	11.148	1.00	58.88	6
ATOM	1685	CD2	LEU	1047	32.610	28.260	11.906	1.00	58.88	6
ATOM	1686	C	LEU	1047	36.307	28.092	9.548	1.00	55.18	6
ATOM	1687	O	LEU	1047	36.106	27.157	8.786	1.00	55.18	8
ATOM	1688	N	TYR	1048	37.283	28.967	9.352	1.00	49.08	7
ATOM	1689	CA	TYR	1048	38.203	28.820	8.234	1.00	49.08	6
ATOM	1690	CB	TYR	1048	39.033	30.097	8.078	1.00	62.53	6
ATOM	1691	CG	TYR	1048	38.422	31.088	7.123	1.00	62.53	6
ATOM	1692	CD1	TYR	1048	37.554	32.092	7.559	1.00	62.53	6
ATOM	1693	CE1	TYR	1048	36.956	32.963	6.644	1.00	62.53	6
ATOM	1694	CD2	TYR	1048	38.678	30.981	5.765	1.00	62.53	6
ATOM	1695	CE2	TYR	1048	38.096	31.829	4.851	1.00	62.53	6
ATOM	1696	CZ	TYR	1048	37.233	32.820	5.280	1.00	62.53	6
ATOM	1697	OH	TYR	1048	36.649	33.642	4.333	1.00	62.53	8
ATOM	1698	C	TYR	1048	39.112	27.618	8.525	1.00	49.08	6

FIG. 3DD

ATOM	1699	O	TYR	1048	39.651	27.008	7.603	1.00	49.08	8
ATOM	1700	N	GLU	1049	39.224	27.293	9.817	1.00	50.97	7
ATOM	1701	CA	GLU	1049	40.047	26.196	10.341	1.00	50.97	6
ATOM	1702	CB	GLU	1049	40.532	26.543	11.761	1.00	95.40	6
ATOM	1703	CG	GLU	1049	41.455	25.483	12.408	1.00	95.40	6
ATOM	1704	CD	GLU	1049	41.583	25.610	13.940	1.00	95.40	6
ATOM	1705	OE1	GLU	1049	41.872	26.717	14.445	1.00	95.40	8
ATOM	1706	OE2	GLU	1049	41.397	24.589	14.641	1.00	95.40	8
ATOM	1707	C	GLU	1049	39.347	24.829	10.395	1.00	50.97	6
ATOM	1708	O	GLU	1049	39.581	23.962	9.543	1.00	50.97	8
ATOM	1709	N	LYS	1050	38.499	24.659	11.416	1.00	80.24	7
ATOM	1710	CA	LYS	1050	37.750	23.420	11.683	1.00	80.24	6
ATOM	1711	CB	LYS	1050	37.217	23.446	13.105	1.00	32.58	6
ATOM	1712	C	LYS	1050	36.603	23.121	10.729	1.00	80.24	6
ATOM	1713	O	LYS	1050	35.910	22.112	10.874	1.00	80.24	8
ATOM	1714	N	LEU	1051	36.394	23.993	9.757	1.00	50.22	7
ATOM	1715	CA	LEU	1051	35.323	23.769	8.810	1.00	50.22	6
ATOM	1716	CB	LEU	1051	34.627	25.081	8.449	1.00	21.77	6
ATOM	1717	CG	LEU	1051	33.258	24.954	7.780	1.00	21.77	6
ATOM	1718	CD1	LEU	1051	32.248	24.632	8.834	1.00	21.77	6
ATOM	1719	CD2	LEU	1051	32.900	26.226	7.065	1.00	21.77	6
ATOM	1720	C	LEU	1051	35.827	23.121	7.540	1.00	50.22	6
ATOM	1721	O	LEU	1051	35.308	22.098	7.123	1.00	50.22	8
ATOM	1722	N	PRO	1052	36.860	23.692	6.913	1.00	73.14	7
ATOM	1723	CD	PRO	1052	37.819	24.695	7.400	1.00	57.36	6
ATOM	1724	CA	PRO	1052	37.372	23.122	5.675	1.00	73.14	6
ATOM	1725	CB	PRO	1052	38.669	23.898	5.460	1.00	57.36	6
ATOM	1726	CG	PRO	1052	38.368	25.214	6.097	1.00	57.36	6
ATOM	1727	C	PRO	1052	37.600	21.638	5.814	1.00	73.14	6
ATOM	1728	O	PRO	1052	36.747	20.823	5.474	1.00	73.14	8
ATOM	1729	N	GLN	1053	38.756	21.308	6.359	1.00	77.10	7
ATOM	1730	CA	GLN	1053	39.139	19.932	6.542	1.00	77.10	6
ATOM	1731	CB	GLN	1053	40.574	19.886	7.003	1.00	100.00	6
ATOM	1732	C	GLN	1053	38.256	19.137	7.504	1.00	77.10	6
ATOM	1733	O	GLN	1053	38.279	17.904	7.479	1.00	77.10	8
ATOM	1734	N	GLY	1054	37.475	19.815	8.341	1.00	78.88	7
ATOM	1735	CA	GLY	1054	36.658	19.075	9.293	1.00	78.88	6
ATOM	1736	C	GLY	1054	35.160	18.960	9.074	1.00	78.88	6
ATOM	1737	O	GLY	1054	34.644	19.099	7.965	1.00	78.88	8
ATOM	1738	N	TYR	1055	34.460	18.683	10.164	1.00	61.80	7
ATOM	1739	CA	TYR	1055	33.018	18.525	10.146	1.00	61.80	6
ATOM	1740	CB	TYR	1055	32.547	17.902	11.458	1.00	100.00	6
ATOM	1741	CG	TYR	1055	32.642	18.897	12.598	1.00	100.00	6
ATOM	1742	CD1	TYR	1055	31.499	19.464	13.161	1.00	100.00	6
ATOM	1743	CE1	TYR	1055	31.592	20.444	14.144	1.00	100.00	6
ATOM	1744	CD2	TYR	1055	33.885	19.337	13.057	1.00	100.00	6
ATOM	1745	CE2	TYR	1055	33.985	20.316	14.039	1.00	100.00	6
ATOM	1746	CZ	TYR	1055	32.835	20.860	14.571	1.00	100.00	6
ATOM	1747	OH	TYR	1055	32.928	21.827	15.531	1.00	100.00	8
ATOM	1748	C	TYR	1055	32.344	19.891	10.001	1.00	61.80	6
ATOM	1749	O	TYR	1055	32.982	20.912	9.728	1.00	61.80	8
ATOM	1750	N	ARG	1056	31.038	19.885	10.231	1.00	78.80	7
ATOM	1751	CA	ARG	1056	30.216	21.079	10.155	1.00	78.80	6
ATOM	1752	CB	ARG	1056	29.674	21.216	8.729	1.00	56.27	6
ATOM	1753	CG	ARG	1056	29.456	19.890	8.001	1.00	56.27	6
ATOM	1754	CD	ARG	1056	29.992	19.943	6.563	1.00	56.27	6
ATOM	1755	NE	ARG	1056	31.444	19.832	6.494	1.00	56.27	7

FIG. 3EE

ATOM	1756	CZ	ARG	1056	32.115	19.413	5.425	1.00	56.27	6
ATOM	1757	NH1	ARG	1056	31.468	19.062	4.323	1.00	56.27	7
ATOM	1758	NH2	ARG	1056	33.441	19.327	5.464	1.00	56.27	7
ATOM	1759	C	ARG	1056	29.074	21.074	11.192	1.00	78.80	6
ATOM	1760	O	ARG	1056	29.031	20.212	12.068	1.00	78.80	8
ATOM	1761	N	LEU	1057	28.149	22.030	11.081	1.00	52.45	7
ATOM	1762	CA	LEU	1057	27.019	22.181	12.016	1.00	52.45	6
ATOM	1763	CB	LEU	1057	25.915	23.018	11.375	1.00	37.29	6
ATOM	1764	CG	LEU	1057	26.218	24.496	11.647	1.00	37.29	6
ATOM	1765	CD1	LEU	1057	25.208	25.439	10.966	1.00	37.29	6
ATOM	1766	CD2	LEU	1057	26.201	24.676	13.134	1.00	37.29	6
ATOM	1767	C	LEU	1057	26.429	20.921	12.635	1.00	52.45	6
ATOM	1768	O	LEU	1057	26.147	19.948	11.957	1.00	52.45	8
ATOM	1769	N	GLU	1058	26.264	20.978	13.955	1.00	65.26	7
ATOM	1770	CA	GLU	1058	25.730	19.856	14.739	1.00	65.26	6
ATOM	1771	CB	GLU	1058	26.251	19.940	16.182	1.00	73.19	6
ATOM	1772	CG	GLU	1058	25.940	21.232	16.943	1.00	73.19	6
ATOM	1773	CD	GLU	1058	26.617	22.490	16.375	1.00	73.19	6
ATOM	1774	OE1	GLU	1058	27.625	22.354	15.641	1.00	73.19	8
ATOM	1775	OE2	GLU	1058	26.158	23.611	16.679	1.00	73.19	8
ATOM	1776	C	GLU	1058	24.207	19.746	14.738	1.00	65.26	6
ATOM	1777	O	GLU	1058	23.497	20.746	14.708	1.00	65.26	8
ATOM	1778	N	LYS	1059	23.721	18.509	14.777	1.00	77.52	7
ATOM	1779	CA	LYS	1059	22.282	18.230	14.756	1.00	77.52	6
ATOM	1780	CB	LYS	1059	22.021	16.720	14.580	1.00	63.67	6
ATOM	1781	CG	LYS	1059	20.563	16.341	14.799	1.00	63.67	6
ATOM	1782	CD	LYS	1059	20.206	15.034	14.104	1.00	63.67	6
ATOM	1783	CE	LYS	1059	20.288	13.847	15.043	1.00	63.67	6
ATOM	1784	NZ	LYS	1059	19.240	13.976	16.098	1.00	63.67	7
ATOM	1785	C	LYS	1059	21.507	18.697	15.978	1.00	77.52	6
ATOM	1786	O	LYS	1059	21.765	18.261	17.093	1.00	77.52	8
ATOM	1787	N	PRO	1060	20.530	19.587	15.780	1.00	65.64	7
ATOM	1788	CD	PRO	1060	20.131	20.220	14.513	1.00	37.22	6
ATOM	1789	CA	PRO	1060	19.725	20.087	16.894	1.00	65.64	6
ATOM	1790	CB	PRO	1060	18.724	21.016	16.219	1.00	37.22	6
ATOM	1791	CG	PRO	1060	19.416	21.473	14.984	1.00	37.22	6
ATOM	1792	C	PRO	1060	19.030	18.898	17.567	1.00	65.64	6
ATOM	1793	O	PRO	1060	18.860	17.840	16.956	1.00	65.64	8
ATOM	1794	N	LEU	1061	18.637	19.074	18.820	1.00	79.51	7
ATOM	1795	CA	LEU	1061	17.962	18.017	19.564	1.00	79.51	6
ATOM	1796	CB	LEU	1061	17.893	18.413	21.044	1.00	82.15	6
ATOM	1797	CG	LEU	1061	17.476	19.851	21.443	1.00	82.15	6
ATOM	1798	CD1	LEU	1061	18.413	20.859	20.777	1.00	82.15	6
ATOM	1799	CD2	LEU	1061	16.033	20.116	21.048	1.00	82.15	6
ATOM	1800	C	LEU	1061	16.562	17.680	19.047	1.00	79.51	6
ATOM	1801	O	LEU	1061	16.187	16.513	19.026	1.00	79.51	8
ATOM	1802	N	ASN	1062	15.802	18.696	18.631	1.00	43.98	7
ATOM	1803	CA	ASN	1062	14.437	18.512	18.124	1.00	43.98	6
ATOM	1804	CB	ASN	1062	13.689	19.843	18.124	1.00	26.42	6
ATOM	1805	CG	ASN	1062	14.462	20.938	17.404	1.00	26.42	6
ATOM	1806	OD1	ASN	1062	15.554	21.327	17.834	1.00	26.42	8
ATOM	1807	ND2	ASN	1062	13.908	21.430	16.294	1.00	26.42	7
ATOM	1808	C	ASN	1062	14.459	17.989	16.718	1.00	43.98	6
ATOM	1809	O	ASN	1062	13.422	17.665	16.156	1.00	43.98	8
ATOM	1810	N	CYS	1063	15.646	17.914	16.143	1.00	48.23	7
ATOM	1811	CA	CYS	1063	15.767	17.460	14.769	1.00	48.23	6
ATOM	1812	CB	CYS	1063	16.914	18.199	14.103	1.00	49.76	6

FIG. 3FF

ATOM	1813	SG	CYS	1063	16.932	17.981	12.363	1.00	49.76	16
ATOM	1814	C	CYS	1063	15.943	15.948	14.559	1.00	48.23	6
ATOM	1815	O	CYS	1063	16.912	15.361	15.039	1.00	48.23	8
ATOM	1816	N	ASP	1064	15.001	15.338	13.834	1.00	41.84	7
ATOM	1817	CA	ASP	1064	15.029	13.907	13.522	1.00	41.84	6
ATOM	1818	CB	ASP	1064	13.788	13.487	12.715	1.00	55.35	6
ATOM	1819	CG	ASP	1064	13.829	12.012	12.290	1.00	55.35	6
ATOM	1820	OD1	ASP	1064	13.977	11.154	13.175	1.00	55.35	8
ATOM	1821	OD2	ASP	1064	13.712	11.710	11.086	1.00	55.35	8
ATOM	1822	C	ASP	1064	16.273	13.599	12.702	1.00	41.84	6
ATOM	1823	O	ASP	1064	16.918	14.521	12.181	1.00	41.84	8
ATOM	1824	N	ASP	1065	16.602	12.309	12.576	1.00	68.56	7
ATOM	1825	CA	ASP	1065	17.789	11.871	11.825	1.00	68.56	6
ATOM	1826	CB	ASP	1065	18.094	10.391	12.086	1.00	100.00	6
ATOM	1827	CG	ASP	1065	18.357	10.088	13.549	1.00	100.00	6
ATOM	1828	OD1	ASP	1065	17.400	10.124	14.341	1.00	100.00	8
ATOM	1829	OD2	ASP	1065	19.524	9.820	13.894	1.00	100.00	8
ATOM	1830	C	ASP	1065	17.654	12.072	10.321	1.00	68.56	6
ATOM	1831	O	ASP	1065	18.627	12.404	9.644	1.00	68.56	8
ATOM	1832	N	GLU	1066	16.457	11.850	9.797	1.00	54.29	7
ATOM	1833	CA	GLU	1066	16.247	12.025	8.378	1.00	54.29	6
ATOM	1834	CB	GLU	1066	14.843	11.583	8.001	1.00	91.86	6
ATOM	1835	CG	GLU	1066	14.550	10.152	8.383	1.00	91.86	6
ATOM	1836	CD	GLU	1066	13.252	9.651	7.787	1.00	91.86	6
ATOM	1837	OE1	GLU	1066	12.729	8.615	8.258	1.00	91.86	8
ATOM	1838	OE2	GLU	1066	12.755	10.296	6.840	1.00	91.86	8
ATOM	1839	C	GLU	1066	16.481	13.479	7.989	1.00	54.29	6
ATOM	1840	O	GLU	1066	17.223	13.758	7.048	1.00	54.29	8
ATOM	1841	N	VAL	1067	15.878	14.408	8.727	1.00	46.62	7
ATOM	1842	CA	VAL	1067	16.032	15.836	8.426	1.00	46.62	6
ATOM	1843	CB	VAL	1067	15.277	16.712	9.430	1.00	20.69	6
ATOM	1844	CG1	VAL	1067	15.286	18.154	8.957	1.00	20.69	6
ATOM	1845	CG2	VAL	1067	13.879	16.208	9.595	1.00	20.69	6
ATOM	1846	C	VAL	1067	17.484	16.314	8.400	1.00	46.62	6
ATOM	1847	O	VAL	1067	17.892	17.076	7.526	1.00	46.62	8
ATOM	1848	N	TYR	1068	18.261	15.858	9.367	1.00	49.64	7
ATOM	1849	CA	TYR	1068	19.654	16.240	9.459	1.00	49.64	6
ATOM	1850	CB	TYR	1068	20.195	15.811	10.813	1.00	42.96	6
ATOM	1851	CG	TYR	1068	21.604	16.239	11.074	1.00	42.96	6
ATOM	1852	CD1	TYR	1068	21.947	17.594	11.093	1.00	42.96	6
ATOM	1853	CE1	TYR	1068	23.236	18.006	11.387	1.00	42.96	6
ATOM	1854	CD2	TYR	1068	22.593	15.301	11.348	1.00	42.96	6
ATOM	1855	CE2	TYR	1068	23.882	15.701	11.640	1.00	42.96	6
ATOM	1856	CZ	TYR	1068	24.198	17.055	11.662	1.00	42.96	6
ATOM	1857	OH	TYR	1068	25.470	17.451	11.985	1.00	42.96	8
ATOM	1858	C	TYR	1068	20.424	15.557	8.338	1.00	49.64	6
ATOM	1859	O	TYR	1068	21.239	16.176	7.663	1.00	49.64	8
ATOM	1860	N	ASP	1069	20.148	14.275	8.144	1.00	54.25	7
ATOM	1861	CA	ASP	1069	20.808	13.495	7.112	1.00	54.25	6
ATOM	1862	CB	ASP	1069	20.056	12.188	6.905	1.00	100.00	6
ATOM	1863	CG	ASP	1069	20.812	11.231	6.043	1.00	100.00	6
ATOM	1864	OD1	ASP	1069	21.225	11.635	4.937	1.00	100.00	8
ATOM	1865	OD2	ASP	1069	20.986	10.076	6.479	1.00	100.00	8
ATOM	1866	C	ASP	1069	20.815	14.279	5.803	1.00	54.25	6
ATOM	1867	O	ASP	1069	21.779	14.247	5.037	1.00	54.25	8
ATOM	1868	N	LEU	1070	19.697	14.956	5.562	1.00	40.31	7
ATOM	1869	CA	LEU	1070	19.496	15.777	4.371	1.00	40.31	6

FIG. 3GG

ATOM	1870	CB	LEU	1070	18.009	16.075	4.195	1.00	25.05	6
ATOM	1871	CG	LEU	1070	17.581	16.966	3.048	1.00	25.05	6
ATOM	1872	CD1	LEU	1070	17.865	16.291	1.720	1.00	25.05	6
ATOM	1873	CD2	LEU	1070	16.114	17.219	3.219	1.00	25.05	6
ATOM	1874	C	LEU	1070	20.290	17.079	4.447	1.00	40.31	6
ATOM	1875	O	LEU	1070	20.561	17.688	3.423	1.00	40.31	8
ATOM	1876	N	MET	1071	20.639	17.510	5.655	1.00	23.05	7
ATOM	1877	CA	MET	1071	21.452	18.703	5.785	1.00	23.05	6
ATOM	1878	CB	MET	1071	21.367	19.310	7.201	1.00	19.93	6
ATOM	1879	CG	MET	1071	20.030	19.910	7.631	1.00	19.93	6
ATOM	1880	SD	MET	1071	20.077	20.344	9.411	1.00	19.93	16
ATOM	1881	CE	MET	1071	18.390	20.649	9.751	1.00	19.93	6
ATOM	1882	C	MET	1071	22.888	18.243	5.504	1.00	23.05	6
ATOM	1883	O	MET	1071	23.591	18.880	4.744	1.00	23.05	8
ATOM	1884	N	ARG	1072	23.319	17.124	6.082	1.00	51.65	7
ATOM	1885	CA	ARG	1072	24.689	16.669	5.864	1.00	51.65	6
ATOM	1886	CB	ARG	1072	24.978	15.434	6.696	1.00	98.84	6
ATOM	1887	CG	ARG	1072	24.870	15.716	8.162	1.00	98.84	6
ATOM	1888	CD	ARG	1072	26.125	16.339	8.727	1.00	98.84	6
ATOM	1889	NE	ARG	1072	27.004	15.305	9.271	1.00	98.84	7
ATOM	1890	CZ	ARG	1072	27.992	15.530	10.131	1.00	98.84	6
ATOM	1891	NH1	ARG	1072	28.232	16.767	10.546	1.00	98.84	7
ATOM	1892	NH2	ARG	1072	28.724	14.521	10.593	1.00	98.84	7
ATOM	1893	C	ARG	1072	25.023	16.404	4.401	1.00	51.65	6
ATOM	1894	O	ARG	1072	26.150	16.659	3.973	1.00	51.65	8
ATOM	1895	N	GLN	1073	24.073	15.900	3.617	1.00	27.54	7
ATOM	1896	CA	GLN	1073	24.376	15.679	2.211	1.00	27.54	6
ATOM	1897	CB	GLN	1073	23.347	14.746	1.568	1.00	67.93	6
ATOM	1898	CG	GLN	1073	21.934	15.149	1.789	1.00	67.93	6
ATOM	1899	CD	GLN	1073	20.972	14.026	1.527	1.00	67.93	6
ATOM	1900	OE1	GLN	1073	20.889	13.066	2.298	1.00	67.93	8
ATOM	1901	NE2	GLN	1073	20.238	14.127	0.422	1.00	67.93	7
ATOM	1902	C	GLN	1073	24.449	17.041	1.500	1.00	27.54	6
ATOM	1903	O	GLN	1073	25.088	17.162	0.453	1.00	27.54	8
ATOM	1904	N	CYS	1074	23.816	18.070	2.072	1.00	36.16	7
ATOM	1905	CA	CYS	1074	23.858	19.423	1.497	1.00	36.16	6
ATOM	1906	CB	CYS	1074	22.925	20.393	2.243	1.00	40.38	6
ATOM	1907	SG	CYS	1074	21.201	20.463	1.797	1.00	40.38	16
ATOM	1908	C	CYS	1074	25.282	19.995	1.627	1.00	36.16	6
ATOM	1909	O	CYS	1074	25.746	20.748	0.767	1.00	36.16	8
ATOM	1910	N	TRP	1075	25.958	19.619	2.716	1.00	26.48	7
ATOM	1911	CA	TRP	1075	27.302	20.120	3.049	1.00	26.48	6
ATOM	1912	CB	TRP	1075	27.413	20.389	4.570	1.00	32.15	6
ATOM	1913	CG	TRP	1075	26.260	21.224	5.181	1.00	32.15	6
ATOM	1914	CD2	TRP	1075	25.679	21.080	6.485	1.00	32.15	6
ATOM	1915	CE2	TRP	1075	24.682	22.075	6.613	1.00	32.15	6
ATOM	1916	CE3	TRP	1075	25.901	20.211	7.553	1.00	32.15	6
ATOM	1917	CD1	TRP	1075	25.607	22.272	4.597	1.00	32.15	6
ATOM	1918	NE1	TRP	1075	24.662	22.783	5.449	1.00	32.15	7
ATOM	1919	CZ2	TRP	1075	23.909	22.222	7.774	1.00	32.15	6
ATOM	1920	CZ3	TRP	1075	25.133	20.361	8.703	1.00	32.15	6
ATOM	1921	CH2	TRP	1075	24.148	21.357	8.807	1.00	32.15	6
ATOM	1922	C	TRP	1075	28.471	19.236	2.622	1.00	26.48	6
ATOM	1923	O	TRP	1075	29.599	19.447	3.071	1.00	26.48	8
ATOM	1924	N	ARG	1076	28.209	18.265	1.751	1.00	51.58	7
ATOM	1925	CA	ARG	1076	29.258	17.367	1.279	1.00	51.58	6
ATOM	1926	CB	ARG	1076	28.683	16.391	0.249	1.00	67.56	6

FIG. 3HH

ATOM	1927	CG	ARG	1076	27.618	15.509	0.847	1.00	67.56	6
ATOM	1928	CD	ARG	1076	27.279	14.291	0.009	1.00	67.56	6
ATOM	1929	NE	ARG	1076	26.267	13.485	0.690	1.00	67.56	7
ATOM	1930	CZ	ARG	1076	25.731	12.365	0.215	1.00	67.56	6
ATOM	1931	NH1	ARG	1076	26.104	11.891	-0.966	1.00	67.56	7
ATOM	1932	NH2	ARG	1076	24.819	11.714	0.929	1.00	67.56	7
ATOM	1933	C	ARG	1076	30.431	18.157	0.710	1.00	51.58	6
ATOM	1934	O	ARG	1076	30.238	19.206	0.103	1.00	51.58	8
ATOM	1935	N	GLU	1077	31.642	17.651	0.941	1.00	50.74	7
ATOM	1936	CA	GLU	1077	32.885	18.281	0.488	1.00	50.74	6
ATOM	1937	CB	GLU	1077	34.059	17.419	0.893	1.00	91.21	6
ATOM	1938	C	GLU	1077	32.927	18.540	-1.013	1.00	50.74	6
ATOM	1939	O	GLU	1077	33.213	19.657	-1.450	1.00	50.74	8
ATOM	1940	N	LYS	1078	32.656	17.494	-1.790	1.00	49.20	7
ATOM	1941	CA	LYS	1078	32.657	17.579	-3.240	1.00	49.20	6
ATOM	1942	CB	LYS	1078	32.895	16.197	-3.847	1.00	93.58	6
ATOM	1943	CG	LYS	1078	34.289	15.666	-3.640	1.00	93.51	6
ATOM	1944	CD	LYS	1078	34.458	14.341	-4.346	1.00	93.51	6
ATOM	1945	CE	LYS	1078	35.872	13.806	-4.191	1.00	93.51	6
ATOM	1946	NZ	LYS	1078	36.025	12.476	-4.860	1.00	93.51	7
ATOM	1947	C	LYS	1078	31.345	18.145	-3.760	1.00	49.20	6
ATOM	1948	O	LYS	1078	30.290	17.528	-3.617	1.00	49.20	8
ATOM	1949	N	PRO	1079	31.390	19.341	-4.366	1.00	30.47	7
ATOM	1950	CD	PRO	1079	32.592	20.190	-4.459	1.00	29.67	6
ATOM	1951	CA	PRO	1079	30.236	20.040	-4.931	1.00	30.47	6
ATOM	1952	CB	PRO	1079	30.887	21.098	-5.791	1.00	29.67	6
ATOM	1953	CG	PRO	1079	32.024	21.511	-4.914	1.00	29.67	6
ATOM	1954	C	PRO	1079	29.235	19.190	-5.711	1.00	30.47	6
ATOM	1955	O	PRO	1079	28.040	19.221	-5.420	1.00	30.47	8
ATOM	1956	N	TYR	1080	29.708	18.462	-6.718	1.00	44.53	7
ATOM	1957	CA	TYR	1080	28.821	17.616	-7.520	1.00	44.53	6
ATOM	1958	CB	TYR	1080	29.576	17.054	-8.730	1.00	62.16	6
ATOM	1959	CG	TYR	1080	30.938	16.479	-8.412	1.00	62.16	6
ATOM	1960	CD1	TYR	1080	31.072	15.207	-7.859	1.00	62.16	6
ATOM	1961	CE1	TYR	1080	32.329	14.691	-7.531	1.00	62.16	6
ATOM	1962	CD2	TYR	1080	32.095	17.223	-8.636	1.00	62.16	6
ATOM	1963	CE2	TYR	1080	33.351	16.722	-8.312	1.00	62.16	6
ATOM	1964	CZ	TYR	1080	33.462	15.458	-7.757	1.00	62.16	6
ATOM	1965	OH	TYR	1080	34.701	14.970	-7.409	1.00	62.16	8
ATOM	1966	C	TYR	1080	28.232	16.490	-6.672	1.00	44.53	6
ATOM	1967	O	TYR	1080	27.282	15.833	-7.087	1.00	44.53	8
ATOM	1968	N	GLU	1081	28.792	16.285	-5.484	1.00	41.53	7
ATOM	1969	CA	GLU	1081	28.285	15.257	-4.588	1.00	41.53	6
ATOM	1970	CB	GLU	1081	29.373	14.767	-3.638	1.00	60.45	6
ATOM	1971	CG	GLU	1081	30.292	13.713	-4.220	1.00	60.45	6
ATOM	1972	CD	GLU	1081	31.240	13.143	-3.182	1.00	60.45	6
ATOM	1973	OE1	GLU	1081	31.903	12.119	-3.470	1.00	60.45	8
ATOM	1974	OE2	GLU	1081	31.323	13.726	-2.079	1.00	60.45	8
ATOM	1975	C	GLU	1081	27.114	15.809	-3.778	1.00	41.53	6
ATOM	1976	O	GLU	1081	26.512	15.099	-2.972	1.00	41.53	8
ATOM	1977	N	ARG	1082	26.812	17.087	-3.975	1.00	50.75	7
ATOM	1978	CA	ARG	1082	25.702	17.706	-3.280	1.00	50.75	6
ATOM	1979	CB	ARG	1082	25.979	19.207	-3.053	1.00	30.76	6
ATOM	1980	CG	ARG	1082	26.429	19.535	-1.624	1.00	30.76	6
ATOM	1981	CD	ARG	1082	27.857	20.100	-1.505	1.00	30.76	6
ATOM	1982	NE	ARG	1082	27.939	21.540	-1.743	1.00	30.76	7
ATOM	1983	CZ	ARG	1082	29.060	22.258	-1.663	1.00	30.76	6

FIG. 3II

ATOM	1984	NH1	ARG	1082	30.225	21.698	-1.358	1.00	30.76	7
ATOM	1985	NH2	ARG	1082	29.007	23.567	-1.865	1.00	30.76	7
ATOM	1986	C	ARG	1082	24.446	17.479	-4.124	1.00	50.75	6
ATOM	1987	O	ARG	1082	24.501	17.497	-5.355	1.00	50.75	8
ATOM	1988	N	PRO	1083	23.303	17.225	-3.464	1.00	42.97	7
ATOM	1989	CD	PRO	1083	23.155	17.153	-1.995	1.00	16.51	6
ATOM	1990	CA	PRO	1083	22.022	16.983	-4.127	1.00	42.97	6
ATOM	1991	CB	PRO	1083	21.171	16.382	-3.015	1.00	16.51	6
ATOM	1992	CG	PRO	1083	21.665	17.079	-1.805	1.00	16.51	6
ATOM	1993	C	PRO	1083	21.450	18.268	-4.715	1.00	42.97	6
ATOM	1994	O	PRO	1083	21.914	19.353	-4.402	1.00	42.97	8
ATOM	1995	N	SER	1084	20.448	18.132	-5.564	1.00	43.29	7
ATOM	1996	CA	SER	1084	19.842	19.275	-6.217	1.00	43.29	6
ATOM	1997	CB	SER	1084	19.553	18.890	-7.643	1.00	28.32	6
ATOM	1998	OG	SER	1084	18.965	17.607	-7.610	1.00	28.32	8
ATOM	1999	C	SER	1084	18.543	19.679	-5.538	1.00	43.29	6
ATOM	2000	O	SER	1084	17.901	18.858	-4.878	1.00	43.29	8
ATOM	2001	N	PHE	1085	18.148	20.934	-5.723	1.00	22.83	7
ATOM	2002	CA	PHE	1085	16.913	21.427	-5.128	1.00	22.83	6
ATOM	2003	CB	PHE	1085	16.688	22.881	-5.538	1.00	7.27	6
ATOM	2004	CG	PHE	1085	17.599	23.814	-4.858	1.00	7.27	6
ATOM	2005	CD1	PHE	1085	18.487	24.598	-5.588	1.00	7.27	6
ATOM	2006	CD2	PHE	1085	17.592	23.899	-3.476	1.00	7.27	6
ATOM	2007	CE1	PHE	1085	19.356	25.462	-4.949	1.00	7.27	6
ATOM	2008	CE2	PHE	1085	18.454	24.756	-2.819	1.00	7.27	6
ATOM	2009	CZ	PHE	1085	19.341	25.545	-3.560	1.00	7.27	6
ATOM	2010	C	PHE	1085	15.710	20.587	-5.510	1.00	22.83	6
ATOM	2011	O	PHE	1085	14.660	20.668	-4.882	1.00	22.83	8
ATOM	2012	N	ALA	1086	15.878	19.789	-6.553	1.00	45.86	7
ATOM	2013	CA	ALA	1086	14.813	18.919	-7.016	1.00	45.86	6
ATOM	2014	CB	ALA	1086	15.037	18.540	-8.430	1.00	15.16	6
ATOM	2015	C	ALA	1086	14.783	17.674	-6.161	1.00	45.86	6
ATOM	2016	O	ALA	1086	13.720	17.175	-5.815	1.00	45.86	8
ATOM	2017	N	GLN	1087	15.959	17.180	-5.810	1.00	32.39	7
ATOM	2018	CA	GLN	1087	16.020	15.990	-5.000	1.00	32.39	6
ATOM	2019	CB	GLN	1087	17.433	15.386	-5.038	1.00	50.88	6
ATOM	2020	CG	GLN	1087	17.971	15.230	-6.466	1.00	50.88	6
ATOM	2021	CD	GLN	1087	19.290	14.488	-6.552	1.00	50.88	6
ATOM	2022	OE1	GLN	1087	20.221	14.752	-5.790	1.00	50.88	8
ATOM	2023	NE2	GLN	1087	19.389	13.577	-7.510	1.00	50.88	7
ATOM	2024	C	GLN	1087	15.617	16.398	-3.592	1.00	32.39	6
ATOM	2025	O	GLN	1087	14.792	15.737	-2.956	1.00	32.39	8
ATOM	2026	N	ILE	1088	16.177	17.507	-3.116	1.00	19.40	7
ATOM	2027	CA	ILE	1088	15.875	17.997	-1.761	1.00	19.40	6
ATOM	2028	CB	ILE	1088	16.519	19.358	-1.532	1.00	20.50	6
ATOM	2029	CG2	ILE	1088	16.172	19.905	-0.185	1.00	20.50	6
ATOM	2030	CG1	ILE	1088	18.017	19.199	-1.630	1.00	20.50	6
ATOM	2031	CD1	ILE	1088	18.747	20.459	-1.361	1.00	20.50	6
ATOM	2032	C	ILE	1088	14.375	18.102	-1.531	1.00	19.40	6
ATOM	2033	O	ILE	1088	13.852	17.646	-0.514	1.00	19.40	8
ATOM	2034	N	LEU	1089	13.697	18.700	-2.500	1.00	31.43	7
ATOM	2035	CA	LEU	1089	12.262	18.860	-2.452	1.00	31.43	6
ATOM	2036	CB	LEU	1089	11.783	19.531	-3.714	1.00	14.58	6
ATOM	2037	CG	LEU	1089	10.376	20.070	-3.576	1.00	14.58	6
ATOM	2038	CD1	LEU	1089	10.208	20.858	-2.288	1.00	14.58	6
ATOM	2039	CD2	LEU	1089	10.136	20.941	-4.788	1.00	14.58	6
ATOM	2040	C	LEU	1089	11.595	17.509	-2.335	1.00	31.43	6

FIG. 3JJ.

ATOM	2041	O	LEU	1089	10.804	17.270	-1.423	1.00	31.43	8
ATOM	2042	N	VAL	1090	11.920	16.619	-3.265	1.00	26.46	7
ATOM	2043	CA	VAL	1090	11.346	15.288	-3.242	1.00	26.46	6
ATOM	2044	CB	VAL	1090	12.042	14.338	-4.171	1.00	24.17	6
ATOM	2045	CG1	VAL	1090	11.419	12.957	-4.012	1.00	24.17	6
ATOM	2046	CG2	VAL	1090	11.913	14.819	-5.581	1.00	24.17	6
ATOM	2047	C	VAL	1090	11.441	14.697	-1.861	1.00	26.46	6
ATOM	2048	O	VAL	1090	10.476	14.126	-1.362	1.00	26.46	8
ATOM	2049	N	SER	1091	12.600	14.819	-1.235	1.00	24.68	7
ATOM	2050	CA	SER	1091	12.726	14.276	0.094	1.00	24.68	6
ATOM	2051	CB	SER	1091	14.156	14.407	0.599	1.00	45.28	6
ATOM	2052	OG	SER	1091	15.039	13.699	-0.249	1.00	45.28	8
ATOM	2053	C	SER	1091	11.742	14.999	1.006	1.00	24.68	6
ATOM	2054	O	SER	1091	10.796	14.379	1.471	1.00	24.68	8
ATOM	2055	N	LEU	1092	11.919	16.302	1.231	1.00	45.44	7
ATOM	2056	CA	LEU	1092	11.001	17.031	2.112	1.00	45.44	6
ATOM	2057	CB	LEU	1092	11.127	18.557	1.905	1.00	19.86	6
ATOM	2058	CG	LEU	1092	12.518	19.144	2.242	1.00	19.86	6
ATOM	2059	CD1	LEU	1092	12.611	20.594	1.810	1.00	19.86	6
ATOM	2060	CD2	LEU	1092	12.793	19.007	3.728	1.00	19.86	6
ATOM	2061	C	LEU	1092	9.554	16.568	1.918	1.00	45.44	6
ATOM	2062	O	LEU	1092	8.821	16.438	2.891	1.00	45.44	8
ATOM	2063	N	ASN	1093	9.162	16.275	0.678	1.00	44.52	7
ATOM	2064	CA	ASN	1093	7.797	15.820	0.360	1.00	44.52	6
ATOM	2065	CB	ASN	1093	7.578	15.906	-1.147	1.00	34.39	6
ATOM	2066	CG	ASN	1093	7.266	17.302	-1.586	1.00	34.39	6
ATOM	2067	OD1	ASN	1093	7.572	17.705	-2.703	1.00	34.39	8
ATOM	2068	ND2	ASN	1093	6.639	18.061	-0.698	1.00	34.39	7
ATOM	2069	C	ASN	1093	7.501	14.414	0.849	1.00	44.52	6
ATOM	2070	O	ASN	1093	6.437	14.137	1.401	1.00	44.52	8
ATOM	2071	N	ARG	1094	8.458	13.529	0.631	1.00	42.85	7
ATOM	2072	CA	ARG	1094	8.329	12.168	1.074	1.00	42.85	6
ATOM	2073	CB	ARG	1094	9.491	11.353	0.472	1.00	83.86	6
ATOM	2074	CG	ARG	1094	10.129	10.325	1.373	1.00	83.62	6
ATOM	2075	CD	ARG	1094	11.099	10.992	2.328	1.00	83.62	6
ATOM	2076	NE	ARG	1094	11.576	10.076	3.359	1.00	83.62	7
ATOM	2077	CZ	ARG	1094	10.787	9.365	4.163	1.00	83.62	6
ATOM	2078	NH1	ARG	1094	9.466	9.461	4.070	1.00	83.62	7
ATOM	2079	NH2	ARG	1094	11.323	8.549	5.061	1.00	83.62	7
ATOM	2080	C	ARG	1094	8.293	12.166	2.628	1.00	42.85	6
ATOM	2081	O	ARG	1094	7.667	11.308	3.239	1.00	42.85	8
ATOM	2082	N	MET	1095	8.934	13.151	3.253	1.00	51.73	7
ATOM	2083	CA	MET	1095	8.991	13.279	4.712	1.00	51.73	6
ATOM	2084	CB	MET	1095	10.206	14.135	5.109	1.00	28.03	6
ATOM	2085	CG	MET	1095	11.242	13.507	5.999	1.00	28.03	6
ATOM	2086	SD	MET	1095	12.707	14.551	6.044	1.00	28.03	16
ATOM	2087	CE	MET	1095	13.094	14.706	4.302	1.00	28.03	6
ATOM	2088	C	MET	1095	7.757	13.989	5.274	1.00	51.73	6
ATOM	2089	O	MET	1095	7.425	13.870	6.450	1.00	51.73	8
ATOM	2090	N	LEU	1096	7.123	14.763	4.413	1.00	48.50	7
ATOM	2091	CA	LEU	1096	5.981	15.557	4.825	1.00	48.50	6
ATOM	2092	CB	LEU	1096	5.889	16.790	3.951	1.00	41.93	6
ATOM	2093	CG	LEU	1096	6.365	18.048	4.638	1.00	41.93	6
ATOM	2094	CD1	LEU	1096	6.177	19.139	3.616	1.00	41.93	6
ATOM	2095	CD2	LEU	1096	5.593	18.342	5.911	1.00	41.93	6
ATOM	2096	C	LEU	1096	4.663	14.859	4.783	1.00	48.50	6
ATOM	2097	O	LEU	1096	3.747	15.199	5.536	1.00	48.50	8

FIG. 3KK

ATOM	2098	N	GLU	1097	4.537	13.900	3.890	1.00	62.96	7
ATOM	2099	CA	GLU	1097	3.261	13.252	3.809	1.00	63.28	6
ATOM	2100	CB	GLU	1097	3.046	12.672	2.424	1.00	90.58	6
ATOM	2101	CG	GLU	1097	2.625	13.708	1.449	1.00	90.58	6
ATOM	2102	CD	GLU	1097	2.523	13.139	0.080	1.00	90.58	6
ATOM	2103	OE1	GLU	1097	3.480	12.481	-0.333	1.00	90.58	8
ATOM	2104	OE2	GLU	1097	1.492	13.317	-0.587	1.00	90.58	8
ATOM	2105	C	GLU	1097	3.099	12.216	4.892	1.00	64.94	6
ATOM	2106	O	GLU	1097	2.839	11.051	4.616	1.00	67.39	8
ATOM	2107	N	GLU	1098	3.279	12.659	6.137	1.00	99.89	7
ATOM	2108	CA	GLU	1098	3.132	11.782	7.288	1.00	99.89	6
ATOM	2109	CB	GLU	1098	4.342	10.880	7.434	1.00	62.46	6
ATOM	2110	CG	GLU	1098	4.908	10.367	6.157	1.00	62.46	6
ATOM	2111	CD	GLU	1098	6.147	9.556	6.415	1.00	62.46	6
ATOM	2112	OE1	GLU	1098	6.614	9.586	7.576	1.00	62.46	8
ATOM	2113	OE2	GLU	1098	6.653	8.914	5.474	1.00	62.46	8
ATOM	2114	C	GLU	1098	2.928	12.540	8.608	1.00	99.89	6
ATOM	2115	O	GLU	1098	1.962	12.277	9.312	1.00	99.89	8
ATOM	2116	N	ARG	1099	3.815	13.483	8.937	1.00	100.00	7
ATOM	2117	CA	ARG	1099	3.735	14.251	10.201	1.00	100.00	6
ATOM	2118	CB	ARG	1099	2.339	14.863	10.443	1.00	95.05	6
ATOM	2119	CG	ARG	1099	2.140	15.416	11.871	1.00	83.68	6
ATOM	2120	CD	ARG	1099	3.239	16.413	12.239	1.00	83.68	6
ATOM	2121	NE	ARG	1099	3.123	16.915	13.609	1.00	83.68	7
ATOM	2122	CZ	ARG	1099	3.314	18.185	13.955	1.00	83.68	6
ATOM	2123	NH1	ARG	1099	3.636	19.072	13.024	1.00	83.68	7
ATOM	2124	NH2	ARG	1099	3.179	18.572	15.222	1.00	83.68	7
ATOM	2125	C	ARG	1099	4.083	13.322	11.354	1.00	100.00	6
ATOM	2126	O	ARG	1099	3.393	13.259	12.370	1.00	100.00	8
ATOM	2127	N	LYS	1100	5.153	12.570	11.174	1.00	88.41	7
ATOM	2128	CA	LYS	1100	5.572	11.681	12.224	1.00	88.41	6
ATOM	2129	CB	LYS	1100	6.250	10.454	11.641	1.00	87.41	6
ATOM	2130	CG	LYS	1100	5.322	9.628	10.762	1.00	87.41	6
ATOM	2131	CD	LYS	1100	3.984	9.336	11.456	1.00	87.41	6
ATOM	2132	CE	LYS	1100	4.165	8.742	12.861	1.00	59.92	6
ATOM	2133	NZ	LYS	1100	4.852	7.411	12.877	1.00	59.92	7
ATOM	2134	C	LYS	1100	6.519	12.453	13.123	1.00	88.41	6
ATOM	2135	O	LYS	1100	7.597	11.969	13.470	1.00	88.41	8
ATOM	2136	N	THR	1101	6.112	13.672	13.472	1.00	100.00	7
ATOM	2137	CA	THR	1101	6.892	14.519	14.356	1.00	100.00	6
ATOM	2138	CB	THR	1101	6.795	13.998	15.811	1.00	100.00	6
ATOM	2139	OG1	THR	1101	5.426	14.034	16.239	1.00	90.24	8
ATOM	2140	OG2	THR	1101	7.652	14.836	16.750	1.00	90.24	6
ATOM	2141	C	THR	1101	8.362	14.565	13.927	1.00	100.00	6
ATOM	2142	O	THR	1101	9.219	13.923	14.541	1.00	100.00	8
ATOM	2143	N	TYR	1102	8.655	15.300	12.862	1.00	39.18	7
ATOM	2144	CA	TYR	1102	10.042	15.411	12.416	1.00	39.18	6
ATOM	2145	CB	TYR	1102	10.106	15.624	10.912	1.00	91.13	6
ATOM	2146	CG	TYR	1102	9.798	14.391	10.132	1.00	60.67	6
ATOM	2147	CD1	TYR	1102	8.500	14.112	9.717	1.00	60.67	6
ATOM	2148	CE1	TYR	1102	8.222	12.956	9.006	1.00	60.67	6
ATOM	2149	CD2	TYR	1102	10.809	13.487	9.821	1.00	60.67	6
ATOM	2150	CE2	TYR	1102	10.544	12.338	9.120	1.00	60.67	6
ATOM	2151	CZ	TYR	1102	9.256	12.078	8.711	1.00	60.67	6
ATOM	2152	OH	TYR	1102	9.019	10.950	7.978	1.00	60.67	8
ATOM	2153	C	TYR	1102	10.781	16.549	13.102	1.00	39.18	6
ATOM	2154	O	TYR	1102	12.003	16.594	13.090	1.00	39.18	8

FIG. 3LL

ATOM	2155	N	VAL	1103	10.028	17.469	13.690	1.00	80.69	7
ATOM	2156	CA	VAL	1103	10.614	18.614	14.370	1.00	80.69	6
ATOM	2157	CB	VAL	1103	10.585	19.857	13.466	1.00	82.85	6
ATOM	2158	CG1	VAL	1103	11.221	21.042	14.165	1.00	25.69	6
ATOM	2159	CG2	VAL	1103	11.310	19.563	12.172	1.00	25.69	6
ATOM	2160	C	VAL	1103	9.791	18.892	15.611	1.00	80.69	6
ATOM	2161	O	VAL	1103	8.677	19.395	15.529	1.00	80.69	8
ATOM	2162	N	ASN	1104	10.345	18.570	16.767	1.00	61.67	7
ATOM	2163	CA	ASN	1104	9.624	18.773	18.003	1.00	61.67	6
ATOM	2164	CB	ASN	1104	10.315	18.015	19.112	1.00	93.99	6
ATOM	2165	CG	ASN	1104	9.344	17.404	20.054	1.00	53.82	6
ATOM	2166	OD1	ASN	1104	8.643	18.111	20.791	1.00	53.82	8
ATOM	2167	ND2	ASN	1104	9.261	16.076	20.028	1.00	53.82	7
ATOM	2168	C	ASN	1104	9.470	20.240	18.395	1.00	61.67	6
ATOM	2169	O	ASN	1104	10.453	20.966	18.484	1.00	61.67	8
ATOM	2170	N	THR	1105	8.233	20.675	18.625	1.00	43.79	7
ATOM	2171	CA	THR	1105	7.960	22.059	19.024	1.00	43.79	6
ATOM	2172	CB	THR	1105	7.081	22.763	18.002	1.00	95.52	6
ATOM	2173	OG1	THR	1105	5.888	22.001	17.786	1.00	51.15	8
ATOM	2174	CG2	THR	1105	7.835	22.923	16.700	1.00	51.15	6
ATOM	2175	C	THR	1105	7.231	22.045	20.350	1.00	43.79	6
ATOM	2176	O	THR	1105	6.598	23.024	20.754	1.00	43.79	8
ATOM	2177	N	THR	1106	7.338	20.905	21.016	1.00	47.73	7
ATOM	2178	CA	THR	1106	6.683	20.671	22.281	1.00	47.73	6
ATOM	2179	CB	THR	1106	5.850	19.415	22.236	1.00	24.03	6
ATOM	2180	OG1	THR	1106	4.835	19.542	21.237	1.00	24.03	8
ATOM	2181	CG2	THR	1106	5.222	19.167	23.580	1.00	24.03	6
ATOM	2182	C	THR	1106	7.676	20.434	23.372	1.00	47.73	6
ATOM	2183	O	THR	1106	8.742	19.880	23.129	1.00	47.73	8
ATOM	2184	N	LEU	1107	7.311	20.833	24.583	1.00	64.31	7
ATOM	2185	CA	LEU	1107	8.174	20.612	25.723	1.00	64.31	6
ATOM	2186	CB	LEU	1107	8.207	21.803	26.637	1.00	96.32	6
ATOM	2187	CG	LEU	1107	8.957	22.900	25.957	1.00	40.62	6
ATOM	2188	CD1	LEU	1107	7.919	23.838	25.432	1.00	40.62	6
ATOM	2189	CD2	LEU	1107	9.864	23.587	26.914	1.00	40.62	6
ATOM	2190	C	LEU	1107	7.795	19.433	26.564	1.00	64.31	6
ATOM	2191	O	LEU	1107	6.801	19.458	27.281	1.00	64.31	8
ATOM	2192	N	TYR	1108	8.708	18.463	26.384	1.00	94.02	7
ATOM	2193	CA	TYR	1108	8.405	17.305	27.238	1.00	94.02	6
ATOM	2194	CB	TYR	1108	8.596	16.009	26.448	1.00	99.65	6
ATOM	2195	CG	TYR	1108	7.705	15.929	25.207	1.00	78.77	6
ATOM	2196	CD1	TYR	1108	7.913	14.643	24.404	1.00	78.77	6
ATOM	2197	CD2	TYR	1108	6.212	15.974	25.538	1.00	78.77	6
ATOM	2198	C	TYR	1108	9.340	17.291	28.449	1.00	94.02	6
ATOM	2199	O	TYR	1108	8.922	16.976	29.574	1.00	94.02	8
ATOM	2200	N	GLU	1109	10.796	17.582	27.521	1.00	92.55	7
ATOM	2201	CA	GLU	1109	11.496	17.815	28.793	1.00	92.55	6
ATOM	2202	CB	GLU	1109	11.234	16.655	29.755	1.00	95.82	6
ATOM	2203	C	GLU	1109	13.002	17.927	28.549	1.00	92.55	6
ATOM	2204	O	GLU	1109	13.672	16.935	28.226	1.00	92.55	8
ATOM	2205	N	LYS	1110	13.581	19.231	28.669	1.00	54.62	7
ATOM	2206	CA	LYS	1110	14.995	19.556	28.430	1.00	54.62	6
ATOM	2207	CB	LYS	1110	15.850	18.294	28.564	1.00	100.00	6
ATOM	2208	CG	LYS	1110	16.129	17.914	30.020	1.00	99.80	6
ATOM	2209	CD	LYS	1110	17.313	16.956	30.171	1.00	99.80	6
ATOM	2210	CE	LYS	1110	17.333	16.240	31.523	1.00	99.80	6
ATOM	2211	NZ	LYS	1110	18.525	15.400	31.710	1.00	99.80	7

FIG. 3MM

ATOM	2212	C	LYS	1110	15.168	20.134	27.023	1.00	54.62	6
ATOM	2213	O	LYS	1110	15.875	19.561	26.181	1.00	54.62	8
ATOM	2214	N	PHE	1111	14.506	21.258	26.825	1.00	53.78	7
ATOM	2215	CA	PHE	1111	14.527	21.994	25.551	1.00	53.78	6
ATOM	2216	CB	PHE	1111	13.134	22.558	25.259	1.00	97.53	6
ATOM	2217	CG	PHE	1111	12.847	22.718	23.764	1.00	42.19	6
ATOM	2218	CD1	PHE	1111	12.368	21.631	23.023	1.00	42.19	6
ATOM	2219	CD2	PHE	1111	13.062	23.951	23.140	1.00	42.19	6
ATOM	2220	CE1	PHE	1111	12.104	21.779	21.655	1.00	42.19	6
ATOM	2221	CE2	PHE	1111	12.798	24.100	21.773	1.00	42.19	6
ATOM	2222	CZ	PHE	1111	12.318	23.013	21.031	1.00	42.19	6
ATOM	2223	C	PHE	1111	15.528	23.149	25.640	1.00	53.78	6
ATOM	2224	O	PHE	1111	15.647	23.812	26.681	1.00	53.78	8
ATOM	2225	N	THR	1112	16.171	23.593	24.331	1.00	41.67	7
ATOM	2226	CA	THR	1112	17.246	24.596	24.296	1.00	41.67	6
ATOM	2227	CB	THR	1112	18.609	23.900	24.280	1.00	81.18	6
ATOM	2228	OG1	THR	1112	18.657	22.952	23.224	1.00	45.38	8
ATOM	2229	CG2	THR	1112	18.915	23.153	25.579	1.00	45.38	6
ATOM	2230	C	THR	1112	17.113	25.461	23.041	1.00	41.67	6
ATOM	2231	O	THR	1112	16.476	25.063	22.055	1.00	41.67	8
ATOM	2232	N	TYR	1113	17.727	26.628	23.125	1.00	88.60	7
ATOM	2233	CA	TYR	1113	17.729	27.614	22.034	1.00	88.60	6
ATOM	2234	CB	TYR	1113	16.857	28.816	22.408	1.00	72.51	6
ATOM	2235	CG	TYR	1113	15.375	28.464	22.561	1.00	11.65	6
ATOM	2236	CD1	TYR	1113	14.778	28.484	23.827	1.00	11.65	6
ATOM	2237	CE1	TYR	1113	13.422	28.166	23.967	1.00	11.65	6
ATOM	2238	CD2	TYR	1113	14.614	28.124	21.435	1.00	11.65	6
ATOM	2239	CE2	TYR	1113	13.258	27.806	21.575	1.00	11.65	6
ATOM	2240	CZ	TYR	1113	12.662	27.827	22.842	1.00	11.65	6
ATOM	2241	OH	TYR	1113	11.344	27.518	22.978	1.00	11.65	8
ATOM	2242	C	TYR	1113	19.155	28.108	21.772	1.00	88.60	6
ATOM	2243	O	TYR	1113	20.133	27.378	21.991	1.00	88.60	8
ATOM	2244	N	ALA	1114	19.217	29.344	21.309	1.00	62.73	7
ATOM	2245	CA	ALA	1114	20.484	30.020	20.989	1.00	62.73	6
ATOM	2246	CB	ALA	1114	21.530	28.992	20.552	1.00	7.22	6
ATOM	2247	C	ALA	1114	20.268	31.024	19.854	1.00	62.73	6
ATOM	2248	O	ALA	1114	20.108	30.642	18.685	1.00	62.73	8
ATOM	2249	N	GLY	1115	20.271	32.287	20.241	1.00	60.96	7
ATOM	2250	CA	GLY	1115	20.078	33.409	19.310	1.00	60.96	6
ATOM	2251	C	GLY	1115	21.034	34.552	19.657	1.00	60.96	6
ATOM	2252	O	GLY	1115	20.817	35.296	20.625	1.00	60.96	8
ATOM	2253	N	ILE	1116	22.069	34.651	18.843	1.00	82.32	7
ATOM	2254	CA	ILE	1116	23.110	35.679	18.992	1.00	82.32	6
ATOM	2255	CB	ILE	1116	22.488	37.073	18.892	1.00	68.50	6
ATOM	2256	C	ILE	1116	23.796	35.537	20.352	1.00	82.32	6
ATOM	2257	O	ILE	1116	24.984	35.192	20.436	1.00	82.32	8
ATOM	2258	OXT	ILE	1116	23.443	36.522	21.208	1.00	64.86	8
TER										
HETATM	2259	C29	TEM	1	14.137	43.777	-1.896	1.00	87.75	6
HETATM	2260	C130	TEM	1	15.517	44.384	-2.200	1.00	92.68	9
HETATM	2261	C31	TEM	1	13.532	43.986	-0.603	1.00	84.61	6
HETATM	2262	C32	TEM	1	10.062	43.539	1.417	1.00	72.29	6
HETATM	2263	C28	TEM	1	13.152	42.505	-7.029	1.00	92.68	6
HETATM	2264	C8	TEM	1	11.669	44.356	4.626	1.00	64.60	6
HETATM	2265	C9	TEM	1	12.234	43.146	5.418	1.00	62.65	6
HETATM	2266	C10	TEM	1	12.979	43.794	6.609	1.00	61.60	6
HETATM	2267	C11	TEM	1	13.328	45.233	6.175	1.00	61.11	6

FIG. 3NN

HETATM	2268	C12	TEM	1	12.788	45.420	4.740	1.00	62.68	6
HETATM	2269	C13	TEM	1	12.175	43.912	2.185	1.00	71.00	6
HETATM	2270	N7	TEM	1	11.303	44.043	3.228	1.00	67.78	7
HETATM	2271	N1	TEM	1	8.672	43.004	-0.559	1.00	73.02	7
HETATM	2272	C2	TEM	1	8.784	43.270	0.784	1.00	71.64	6
HETATM	2273	N3	TEM	1	7.669	43.306	1.546	1.00	71.42	7
HETATM	2274	C4	TEM	1	7.718	43.568	2.851	1.00	69.68	6
HETATM	2275	N5	TEM	1	8.853	43.811	3.473	1.00	68.84	7
HETATM	2276	C6	TEM	1	10.030	43.817	2.820	1.00	69.92	6
HETATM	2277	C14	TEM	1	11.530	43.630	1.036	1.00	75.68	6
HETATM	2278	O22	TEM	1	13.956	40.236	-4.115	1.00	92.68	8
HETATM	2279	C23	TEM	1	13.420	41.285	-6.355	1.00	92.68	6
HETATM	2280	C24	TEM	1	12.844	40.071	-6.856	1.00	92.68	6
HETATM	2281	C25	TEM	1	12.014	40.102	-8.027	1.00	92.68	6
HETATM	2282	C26	TEM	1	11.757	41.334	-8.689	1.00	92.68	6
HETATM	2283	C27	TEM	1	12.330	42.534	-8.187	1.00	92.68	6
HETATM	2284	O21	TEM	1	15.786	41.592	-5.276	1.00	92.68	8
HETATM	2285	C15	TEM	1	12.216	43.429	-0.313	1.00	80.63	6
HETATM	2286	C16	TEM	1	11.576	42.675	-1.308	1.00	83.45	6
HETATM	2287	C17	TEM	1	12.141	42.492	-2.551	1.00	87.27	6
HETATM	2288	C18	TEM	1	13.399	43.018	-2.887	1.00	88.78	6
HETATM	2289	N19	TEM	1	13.818	42.732	-4.220	1.00	90.27	7
HETATM	2290	S20	TEM	1	14.444	41.335	-4.875	1.00	92.68	16
ATOM	2291	S	SO4	2	25.361	40.893	-8.736	1.00	15.55	16
ATOM	2292	O1	SO4	2	26.331	39.742	-8.499	1.00	20.26	8
ATOM	2293	O2	SO4	2	25.230	41.131	-10.222	1.00	12.30	8
ATOM	2294	O3	SO4	2	23.982	40.607	-8.171	1.00	16.39	8
ATOM	2295	O4	SO4	2	25.930	42.110	-8.051	1.00	17.72	8

END

FIG. 300

ATOM	1	N	VAL	A	818	77.669	47.027	2.354	1.00	20.00
ATOM	2	CA	VAL	A	818	76.422	47.479	1.690	1.00	20.00
ATOM	3	C	VAL	A	818	75.257	46.471	1.737	1.00	20.00
ATOM	4	O	VAL	A	818	75.361	45.363	2.335	1.00	20.00
ATOM	5	CB	VAL	A	818	76.716	47.863	0.250	1.00	20.00
ATOM	9	N	LEU	A	819	74.145	46.870	1.095	1.00	20.00
ATOM	10	CA	LEU	A	819	72.922	46.055	1.058	1.00	20.00
ATOM	11	C	LEU	A	819	72.341	45.959	-0.347	1.00	20.00
ATOM	12	O	LEU	A	819	71.187	46.223	-0.571	1.00	20.00
ATOM	13	CB	LEU	A	819	71.897	46.637	2.052	1.00	20.00
ATOM	14	CG	LEU	A	819	70.399	46.340	1.987	1.00	20.00
ATOM	15	CD1	LEU	A	819	70.026	45.327	3.039	1.00	20.00
ATOM	16	CD2	LEU	A	819	69.612	47.643	2.186	1.00	20.00
ATOM	18	N	ASP	A	820	73.165	45.565	-1.294	1.00	20.00
ATOM	19	CA	ASP	A	820	72.758	45.427	-2.685	1.00	20.00
ATOM	20	C	ASP	A	820	71.419	45.961	-3.188	1.00	20.00
ATOM	21	O	ASP	A	820	70.510	45.182	-3.445	1.00	20.00
ATOM	22	CB	ASP	A	820	72.867	43.971	-3.103	1.00	20.00
ATOM	23	CG	ASP	A	820	72.637	43.799	-4.570	1.00	20.00
ATOM	24	OD1	ASP	A	820	72.617	42.622	-5.045	1.00	20.00
ATOM	25	OD2	ASP	A	820	72.468	44.861	-5.242	1.00	20.00
ATOM	27	N	TRP	A	821	71.336	47.280	-3.390	1.00	20.00
ATOM	28	CA	TRP	A	821	70.128	47.958	-3.916	1.00	20.00
ATOM	29	C	TRP	A	821	69.296	47.063	-4.814	1.00	20.00
ATOM	30	O	TRP	A	821	68.077	47.237	-4.938	1.00	20.00
ATOM	31	CB	TRP	A	821	70.479	49.190	-4.782	1.00	20.00
ATOM	32	CG	TRP	A	821	69.336	50.211	-4.771	1.00	20.00
ATOM	33	CD1	TRP	A	821	68.872	50.892	-3.675	1.00	20.00
ATOM	34	CD2	TRP	A	821	68.465	50.552	-5.841	1.00	20.00
ATOM	35	NE1	TRP	A	821	67.753	51.628	-4.001	1.00	20.00
ATOM	36	CE2	TRP	A	821	67.482	51.435	-5.325	1.00	20.00
ATOM	37	CE3	TRP	A	821	68.408	50.201	-7.177	1.00	20.00
ATOM	38	CZ2	TRP	A	821	66.462	51.963	-6.104	1.00	20.00
ATOM	39	CZ3	TRP	A	821	67.382	50.730	-7.962	1.00	20.00
ATOM	40	CH2	TRP	A	821	66.430	51.597	-7.420	1.00	20.00
ATOM	43	N	ASN	A	822	69.999	46.156	-5.498	1.00	20.00
ATOM	44	CA	ASN	A	822	69.370	45.213	-6.404	1.00	20.00
ATOM	45	C	ASN	A	822	67.947	44.823	-5.911	1.00	20.00
ATOM	46	O	ASN	A	822	67.000	44.734	-6.707	1.00	20.00
ATOM	47	CB	ASN	A	822	70.291	43.986	-6.531	1.00	20.00
ATOM	48	CG	ASN	A	822	69.610	42.766	-7.181	1.00	20.00
ATOM	49	OD1	ASN	A	822	69.287	42.766	-8.393	1.00	20.00
ATOM	50	ND2	ASN	A	822	69.406	41.706	-6.377	1.00	20.00
ATOM	54	N	ASP	A	823	67.778	44.632	-4.602	1.00	20.00
ATOM	55	CA	ASP	A	823	66.472	44.212	-4.129	1.00	20.00
ATOM	56	C	ASP	A	823	65.921	44.808	-2.847	1.00	20.00
ATOM	57	O	ASP	A	823	66.179	44.295	-1.758	1.00	20.00
ATOM	58	CB	ASP	A	823	66.454	42.681	-4.008	1.00	20.00
ATOM	60	N	ILE	A	824	65.166	45.894	-2.988	1.00	20.00
ATOM	61	CA	ILE	A	824	64.480	46.524	-1.859	1.00	20.00
ATOM	62	C	ILE	A	824	63.021	46.501	-2.412	1.00	20.00
ATOM	63	O	ILE	A	824	62.776	46.906	-3.570	1.00	20.00
ATOM	64	CB	ILE	A	824	64.955	48.019	-1.586	1.00	20.00
ATOM	65	CG1	ILE	A	824	65.666	48.576	-2.803	1.00	20.00
ATOM	66	CG2	ILE	A	824	65.845	48.113	-0.382	1.00	20.00
ATOM	67	CD1	ILE	A	824	67.135	48.549	-2.681	1.00	20.00

FIG. 4A

ATOM	69	N	LYS	A	825	62.077	45.969	-1.626	1.00	20.00
ATOM	70	CA	LYS	A	825	60.645	45.921	-2.029	1.00	20.00
ATOM	71	C	LYS	A	825	59.922	47.060	-1.266	1.00	20.00
ATOM	72	O	LYS	A	825	59.578	46.946	-0.097	1.00	20.00
ATOM	73	CB	LYS	A	825	60.043	44.561	-1.696	1.00	20.00
ATOM	75	N	PHE	A	826	59.696	48.147	-1.988	1.00	20.00
ATOM	76	CA	PHE	A	826	59.153	49.401	-1.462	1.00	20.00
ATOM	77	C	PHE	A	826	57.643	49.569	-1.593	1.00	20.00
ATOM	78	O	PHE	A	826	57.160	50.073	-2.593	1.00	20.00
ATOM	79	CB	PHE	A	826	59.882	50.481	-2.224	1.00	20.00
ATOM	80	CG	PHE	A	826	60.298	50.013	-3.604	1.00	20.00
ATOM	81	CD1	PHE	A	826	59.336	49.841	-4.613	1.00	20.00
ATOM	82	CD2	PHE	A	826	61.611	49.711	-3.887	1.00	20.00
ATOM	83	CE1	PHE	A	826	59.675	49.383	-5.876	1.00	20.00
ATOM	84	CE2	PHE	A	826	61.960	49.249	-5.145	1.00	20.00
ATOM	85	CZ	PHE	A	826	60.984	49.086	-6.144	1.00	20.00
ATOM	87	N	GLN	A	827	56.919	49.173	-0.550	1.00	20.00
ATOM	88	CA	GLN	A	827	55.459	49.206	-0.491	1.00	20.00
ATOM	89	C	GLN	A	827	54.788	50.547	-0.268	1.00	20.00
ATOM	90	O	GLN	A	827	54.134	51.071	-1.177	1.00	20.00
ATOM	91	CB	GLN	A	827	54.978	48.268	0.591	1.00	20.00
ATOM	92	CG	GLN	A	827	56.111	47.581	1.340	1.00	20.00
ATOM	93	CD	GLN	A	827	56.511	46.315	0.637	1.00	20.00
ATOM	94	OE1	GLN	A	827	56.636	45.253	1.256	1.00	20.00
ATOM	95	NE2	GLN	A	827	56.688	46.410	-0.675	1.00	20.00
ATOM	99	N	ASP	A	828	54.918	51.103	0.928	1.00	20.00
ATOM	100	CA	ASP	A	828	54.261	52.360	1.165	1.00	20.00
ATOM	101	C	ASP	A	828	54.815	53.309	2.231	1.00	20.00
ATOM	102	O	ASP	A	828	55.694	52.973	3.033	1.00	20.00
ATOM	103	CB	ASP	A	828	52.856	52.049	1.499	1.00	20.00
ATOM	104	CG	ASP	A	828	52.783	50.948	2.460	1.00	20.00
ATOM	105	OD1	ASP	A	828	52.099	49.943	2.182	1.00	20.00
ATOM	106	OD2	ASP	A	828	53.439	51.088	3.504	1.00	20.00
ATOM	108	N	VAL	A	829	54.278	54.522	2.216	1.00	20.00
ATOM	109	CA	VAL	A	829	54.681	55.525	3.158	1.00	20.00
ATOM	110	C	VAL	A	829	54.405	54.794	4.471	1.00	20.00
ATOM	111	O	VAL	A	829	53.373	54.176	4.562	1.00	20.00
ATOM	112	CB	VAL	A	829	53.772	56.742	2.971	1.00	20.00
ATOM	114	N	ILE	A	830	55.298	54.759	5.453	1.00	20.00
ATOM	115	CA	ILE	A	830	54.911	54.062	6.686	1.00	20.00
ATOM	116	C	ILE	A	830	54.690	55.170	7.627	1.00	20.00
ATOM	117	O	ILE	A	830	55.296	55.229	8.696	1.00	20.00
ATOM	118	CB	ILE	A	830	56.004	53.170	7.366	1.00	20.00
ATOM	119	CG1	ILE	A	830	56.458	52.054	6.437	1.00	20.00
ATOM	120	CG2	ILE	A	830	55.435	52.493	8.636	1.00	20.00
ATOM	121	CD1	ILE	A	830	57.626	51.361	6.996	1.00	20.00
ATOM	123	N	GLY	A	831	53.802	56.059	7.244	1.00	20.00
ATOM	124	CA	GLY	A	831	53.588	57.205	8.087	1.00	20.00
ATOM	125	C	GLY	A	831	54.694	58.162	7.693	1.00	20.00
ATOM	126	O	GLY	A	831	55.359	57.972	6.691	1.00	20.00
ATOM	128	N	GLU	A	832	54.888	59.180	8.505	1.00	20.00
ATOM	129	CA	GLU	A	832	55.889	60.205	8.260	1.00	20.00
ATOM	130	C	GLU	A	832	57.146	59.876	7.452	1.00	20.00
ATOM	131	O	GLU	A	832	57.220	58.893	6.667	1.00	20.00
ATOM	132	CB	GLU	A	832	56.346	60.832	9.592	1.00	20.00
ATOM	133	CG	GLU	A	832	56.473	62.337	9.489	1.00	20.00
ATOM	134	CD	GLU	A	832	55.501	62.908	8.468	1.00	20.00

FIG. 4B

ATOM	135	OE1	GLU	A	832	54.643	63.721	8.897	1.00	20.00
ATOM	136	OE2	GLU	A	832	55.599	62.524	7.266	1.00	20.00
ATOM	138	N	GLY	A	833	58.134	60.754	7.680	1.00	20.00
ATOM	139	CA	GLY	A	833	59.440	60.670	7.054	1.00	20.00
ATOM	140	C	GLY	A	833	60.222	61.871	7.561	1.00	20.00
ATOM	141	O	GLY	A	833	60.606	61.957	8.770	1.00	20.00
ATOM	143	N	ASN	A	834	60.380	62.816	6.621	1.00	20.00
ATOM	144	CA	ASN	A	834	61.123	64.085	6.772	1.00	20.00
ATOM	145	C	ASN	A	834	62.555	63.797	7.139	1.00	20.00
ATOM	146	O	ASN	A	834	62.796	63.133	8.141	1.00	20.00
ATOM	147	CB	ASN	A	834	60.584	65.052	7.859	1.00	20.00
ATOM	148	CG	ASN	A	834	61.664	66.125	8.258	1.00	20.00
ATOM	149	OD1	ASN	A	834	61.998	66.999	7.444	1.00	20.00
ATOM	150	ND2	ASN	A	834	62.224	66.022	9.491	1.00	20.00
ATOM	154	N	PHE	A	835	63.474	64.373	6.355	1.00	20.00
ATOM	155	CA	PHE	A	835	64.922	64.216	6.526	1.00	20.00
ATOM	156	C	PHE	A	835	64.972	63.040	7.488	1.00	20.00
ATOM	157	O	PHE	A	835	65.560	63.063	8.616	1.00	20.00
ATOM	158	CB	PHE	A	835	65.545	65.547	7.028	1.00	20.00
ATOM	159	CG	PHE	A	835	65.828	66.560	5.895	1.00	20.00
ATOM	160	CD1	PHE	A	835	65.442	67.913	6.013	1.00	20.00
ATOM	161	CD2	PHE	A	835	66.534	66.176	4.742	1.00	20.00
ATOM	162	CE1	PHE	A	835	65.761	68.870	5.004	1.00	20.00
ATOM	163	CE2	PHE	A	835	66.859	67.138	3.725	1.00	20.00
ATOM	164	CZ	PHE	A	835	66.469	68.482	3.867	1.00	20.00
ATOM	166	N	GLY	A	836	64.251	62.029	6.984	1.00	20.00
ATOM	167	CA	GLY	A	836	64.025	60.759	7.647	1.00	20.00
ATOM	168	C	GLY	A	836	62.817	60.226	6.884	1.00	20.00
ATOM	169	O	GLY	A	836	61.874	59.661	7.452	1.00	20.00
ATOM	171	N	GLN	A	837	62.827	60.432	5.571	1.00	20.00
ATOM	172	CA	GLN	A	837	61.720	59.959	4.749	1.00	20.00
ATOM	173	C	GLN	A	837	61.471	58.496	5.132	1.00	20.00
ATOM	174	O	GLN	A	837	62.278	57.647	4.742	1.00	20.00
ATOM	175	CB	GLN	A	837	62.112	60.066	3.253	1.00	20.00
ATOM	176	CG	GLN	A	837	63.459	60.807	2.984	1.00	20.00
ATOM	177	CD	GLN	A	837	63.541	61.552	1.605	1.00	20.00
ATOM	178	OE1	GLN	A	837	64.298	62.539	1.447	1.00	20.00
ATOM	179	NE2	GLN	A	837	62.786	61.053	0.607	1.00	20.00
ATOM	183	N	VAL	A	838	60.400	58.162	5.872	1.00	20.00
ATOM	184	CA	VAL	A	838	60.233	56.718	6.211	1.00	20.00
ATOM	185	C	VAL	A	838	59.296	55.833	5.400	1.00	20.00
ATOM	186	O	VAL	A	838	58.143	55.705	5.734	1.00	20.00
ATOM	187	CB	VAL	A	838	59.824	56.442	7.659	1.00	20.00
ATOM	188	CG1	VAL	A	838	60.786	55.456	8.230	1.00	20.00
ATOM	189	CG2	VAL	A	838	59.760	57.703	8.475	1.00	20.00
ATOM	191	N	LEU	A	839	59.820	55.181	4.373	1.00	20.00
ATOM	192	CA	LEU	A	839	59.031	54.306	3.542	1.00	20.00
ATOM	193	C	LEU	A	839	58.983	52.882	4.069	1.00	20.00
ATOM	194	O	LEU	A	839	59.676	52.547	5.015	1.00	20.00
ATOM	195	CB	LEU	A	839	59.566	54.385	2.111	1.00	20.00
ATOM	196	CG	LEU	A	839	58.912	55.608	1.396	1.00	20.00
ATOM	197	CD1	LEU	A	839	58.295	56.545	2.426	1.00	20.00
ATOM	198	CD2	LEU	A	839	59.886	56.367	0.533	1.00	20.00
ATOM	200	N	LYS	A	840	58.119	52.049	3.503	1.00	20.00
ATOM	201	CA	LYS	A	840	58.031	50.646	3.945	1.00	20.00
ATOM	202	C	LYS	A	840	58.687	49.724	2.927	1.00	20.00
ATOM	203	O	LYS	A	840	58.645	49.971	1.725	1.00	20.00

FIG. 4C

ATOM	204	CB	LYS	A	840	56.577	50.198	4.145	1.00	20.00
ATOM	205	CG	LYS	A	840	56.445	49.166	5.251	1.00	20.00
ATOM	206	CD	LYS	A	840	55.843	47.830	4.789	1.00	20.00
ATOM	207	CE	LYS	A	840	55.173	47.110	5.960	1.00	20.00
ATOM	208	NZ	LYS	A	840	56.154	46.444	6.801	1.00	20.00
ATOM	213	N	ALA	A	841	59.302	48.650	3.383	1.00	20.00
ATOM	214	CA	ALA	A	841	59.929	47.798	2.393	1.00	20.00
ATOM	215	C	ALA	A	841	60.199	46.360	2.787	1.00	20.00
ATOM	216	O	ALA	A	841	60.460	46.044	3.971	1.00	20.00
ATOM	217	CB	ALA	A	841	61.224	48.462	1.884	1.00	20.00
ATOM	219	N	ARG	A	842	60.111	45.506	1.759	1.00	20.00
ATOM	220	CA	ARG	A	842	60.347	44.075	1.824	1.00	20.00
ATOM	221	C	ARG	A	842	61.797	43.918	1.340	1.00	20.00
ATOM	222	O	ARG	A	842	62.105	43.967	0.158	1.00	20.00
ATOM	223	CB	ARG	A	842	59.365	43.360	0.902	1.00	20.00
ATOM	225	N	ILE	A	843	62.688	43.746	2.293	1.00	20.00
ATOM	226	CA	ILE	A	843	64.113	43.638	2.034	1.00	20.00
ATOM	227	C	ILE	A	843	64.747	42.223	2.205	1.00	20.00
ATOM	228	O	ILE	A	843	64.527	41.503	3.201	1.00	20.00
ATOM	229	CB	ILE	A	843	64.846	44.662	2.928	1.00	20.00
ATOM	230	CG1	ILE	A	843	65.867	45.411	2.103	1.00	20.00
ATOM	231	CG2	ILE	A	843	65.469	43.996	4.130	1.00	20.00
ATOM	232	CD1	ILE	A	843	66.176	44.779	0.772	1.00	20.00
ATOM	234	N	LYS	A	844	65.549	41.837	1.226	1.00	20.00
ATOM	235	CA	LYS	A	844	66.190	40.551	1.273	1.00	20.00
ATOM	236	C	LYS	A	844	67.652	40.641	1.709	1.00	20.00
ATOM	237	O	LYS	A	844	68.540	40.820	0.869	1.00	20.00
ATOM	238	CB	LYS	A	844	66.093	39.875	-0.111	1.00	20.00
ATOM	240	N	LYS	A	845	67.897	40.510	3.014	1.00	20.00
ATOM	241	CA	LYS	A	845	69.261	40.516	3.545	1.00	20.00
ATOM	242	C	LYS	A	845	69.917	39.112	3.335	1.00	20.00
ATOM	243	O	LYS	A	845	69.306	38.060	3.678	1.00	20.00
ATOM	244	CB	LYS	A	845	69.255	40.857	5.035	1.00	20.00
ATOM	246	N	ASP	A	846	71.148	39.140	2.765	1.00	20.00
ATOM	247	CA	ASP	A	846	72.022	37.977	2.481	1.00	20.00
ATOM	248	C	ASP	A	846	71.224	36.671	2.559	1.00	20.00
ATOM	249	O	ASP	A	846	71.231	35.953	3.581	1.00	20.00
ATOM	250	CB	ASP	A	846	73.214	37.987	3.484	1.00	20.00
ATOM	251	CG	ASP	A	846	74.448	37.141	3.002	1.00	20.00
ATOM	252	OD1	ASP	A	846	74.788	37.167	1.784	1.00	20.00
ATOM	253	OD2	ASP	A	846	75.078	36.450	3.869	1.00	20.00
ATOM	255	N	GLY	A	847	70.497	36.405	1.476	1.00	20.00
ATOM	256	CA'	GLY	A	847	69.670	35.206	1.405	1.00	20.00
ATOM	257	C	GLY	A	847	68.642	35.071	2.527	1.00	20.00
ATOM	258	O	GLY	A	847	68.972	34.604	3.636	1.00	20.00
ATOM	260	N	LEU	A	848	67.406	35.481	2.198	1.00	20.00
ATOM	261	CA	LEU	A	848	66.192	35.495	3.049	1.00	20.00
ATOM	262	C	LEU	A	848	65.707	36.956	3.333	1.00	20.00
ATOM	263	O	LEU	A	848	66.470	37.844	3.751	1.00	20.00
ATOM	264	CB	LEU	A	848	66.402	34.666	4.318	1.00	20.00
ATOM	265	CG	LEU	A	848	66.559	35.338	5.653	1.00	20.00
ATOM	266	CD1	LEU	A	848	66.241	34.369	6.804	1.00	20.00
ATOM	267	CD2	LEU	A	848	68.011	35.849	5.755	1.00	20.00
ATOM	269	N	ARG	A	849	64.434	37.188	3.011	1.00	20.00
ATOM	270	CA	ARG	A	849	63.793	38.491	3.149	1.00	20.00
ATOM	271	C	ARG	A	849	63.495	38.916	4.576	1.00	20.00
ATOM	272	O	ARG	A	849	63.795	38.195	5.542	1.00	20.00

FIG. 4D

ATOM	273	CB	ARG	A	849	62.465	38.508	2.388	1.00	20.00
ATOM	274	CG	ARG	A	849	62.570	38.136	0.936	1.00	20.00
ATOM	275	CD	ARG	A	849	61.348	38.648	0.182	1.00	20.00
ATOM	276	NE	ARG	A	849	61.060	37.918	-1.060	1.00	20.00
ATOM	277	CZ	ARG	A	849	60.337	36.795	-1.117	1.00	20.00
ATOM	278	NH1	ARG	A	849	59.833	36.281	0.018	1.00	20.00
ATOM	279	NH2	ARG	A	849	60.113	36.198	-2.308	1.00	20.00
ATOM	286	N	MET	A	850	62.903	40.112	4.678	1.00	20.00
ATOM	287	CA	MET	A	850	62.466	40.710	5.938	1.00	20.00
ATOM	288	C	MET	A	850	61.786	42.087	5.756	1.00	20.00
ATOM	289	O	MET	A	850	61.816	42.702	4.694	1.00	20.00
ATOM	290	CB	MET	A	850	63.628	40.814	6.953	1.00	20.00
ATOM	291	CG	MET	A	850	65.005	41.061	6.376	1.00	20.00
ATOM	292	SD	MET	A	850	66.205	41.855	7.507	1.00	20.00
ATOM	293	CE	MET	A	850	66.021	40.869	9.036	1.00	20.00
ATOM	295	N	ASP	A	851	61.105	42.523	6.800	1.00	20.00
ATOM	296	CA	ASP	A	851	60.477	43.812	6.787	1.00	20.00
ATOM	297	C	ASP	A	851	61.586	44.780	7.213	1.00	20.00
ATOM	298	O	ASP	A	851	62.559	44.403	7.904	1.00	20.00
ATOM	299	CB	ASP	A	851	59.381	43.909	7.855	1.00	20.00
ATOM	300	CG	ASP	A	851	58.154	43.076	7.546	1.00	20.00
ATOM	301	OD1	ASP	A	851	57.886	42.769	6.352	1.00	20.00
ATOM	302	OD2	ASP	A	851	57.452	42.744	8.545	1.00	20.00
ATOM	304	N	ALA	A	852	61.366	46.044	6.842	1.00	20.00
ATOM	305	CA	ALA	A	852	62.230	47.173	7.161	1.00	20.00
ATOM	306	C	ALA	A	852	61.483	48.457	6.814	1.00	20.00
ATOM	307	O	ALA	A	852	60.631	48.480	5.902	1.00	20.00
ATOM	308	CB	ALA	A	852	63.507	47.092	6.332	1.00	20.00
ATOM	310	N	ALA	A	853	61.774	49.522	7.546	1.00	20.00
ATOM	311	CA	ALA	A	853	61.205	50.818	7.189	1.00	20.00
ATOM	312	C	ALA	A	853	62.439	51.427	6.518	1.00	20.00
ATOM	313	O	ALA	A	853	63.529	50.919	6.771	1.00	20.00
ATOM	314	CB	ALA	A	853	60.812	51.581	8.418	1.00	20.00
ATOM	316	N	ILE	A	854	62.300	52.470	5.685	1.00	20.00
ATOM	317	CA	ILE	A	854	63.436	53.072	4.960	1.00	20.00
ATOM	318	C	ILE	A	854	63.501	54.570	5.142	1.00	20.00
ATOM	319	O	ILE	A	854	62.478	55.156	5.413	1.00	20.00
ATOM	320	CB	ILE	A	854	63.313	52.777	3.457	1.00	20.00
ATOM	321	CG1	ILE	A	854	63.527	51.284	3.195	1.00	20.00
ATOM	322	CG2	ILE	A	854	64.353	53.554	2.664	1.00	20.00
ATOM	323	CD1	ILE	A	854	64.906	50.722	3.717	1.00	20.00
ATOM	325	N	LYS	A	855	64.699	55.189	5.023	1.00	20.00
ATOM	326	CA	LYS	A	855	64.901	56.684	5.158	1.00	20.00
ATOM	327	C	LYS	A	855	65.800	57.286	4.079	1.00	20.00
ATOM	328	O	LYS	A	855	65.740	56.867	2.946	1.00	20.00
ATOM	329	CB	LYS	A	855	65.417	57.088	6.580	1.00	20.00
ATOM	330	CG	LYS	A	855	66.949	57.267	6.792	1.00	20.00
ATOM	331	CD	LYS	A	855	67.333	57.776	8.262	1.00	20.00
ATOM	332	CE	LYS	A	855	68.597	57.022	8.917	1.00	20.00
ATOM	333	NZ	LYS	A	855	69.828	57.804	9.506	1.00	20.00
ATOM	338	N	ARG	A	856	66.573	58.311	4.439	1.00	20.00
ATOM	339	CA	ARG	A	856	67.569	59.035	3.573	1.00	20.00
ATOM	340	C	ARG	A	856	66.957	60.199	2.856	1.00	20.00
ATOM	341	O	ARG	A	856	66.375	60.027	1.793	1.00	20.00
ATOM	342	CB	ARG	A	856	68.288	58.135	2.533	1.00	20.00
ATOM	343	CG	ARG	A	856	69.278	58.948	1.706	1.00	20.00
ATOM	344	CD	ARG	A	856	68.965	58.943	0.179	1.00	20.00

FIG. 4E

ATOM	345	NE	ARG	A	856	68.880	60.276	-0.435	1.00	20.00
ATOM	346	CZ	ARG	A	856	68.623	60.497	-1.732	1.00	20.00
ATOM	347	NH1	ARG	A	856	68.425	59.484	-2.568	1.00	20.00
ATOM	348	NH2	ARG	A	856	68.555	61.750	-2.204	1.00	20.00
ATOM	355	N	MET	A	857	67.166	61.381	3.446	1.00	20.00
ATOM	356	CA	MET	A	857	66.581	62.674	2.991	1.00	20.00
ATOM	357	C	MET	A	857	67.495	63.831	2.508	1.00	20.00
ATOM	358	O	MET	A	857	68.427	64.269	3.254	1.00	20.00
ATOM	359	CB	MET	A	857	65.682	63.220	4.125	1.00	20.00
ATOM	360	CG	MET	A	857	64.287	63.699	3.730	1.00	20.00
ATOM	361	SD	MET	A	857	62.819	63.037	4.735	1.00	20.00
ATOM	362	CE	MET	A	857	61.431	64.067	3.876	1.00	20.00
ATOM	363	OXT	MET	A	857	67.199	64.316	1.383	1.00	20.00
ATOM	365	N	ASP	A	864	77.202	66.313	-0.527	1.00	20.00
ATOM	366	CA	ASP	A	864	77.838	67.381	-1.394	1.00	20.00
ATOM	367	C	ASP	A	864	78.591	68.418	-0.580	1.00	20.00
ATOM	368	O	ASP	A	864	79.619	68.925	-1.043	1.00	20.00
ATOM	369	CB	ASP	A	864	76.768	68.105	-2.272	1.00	20.00
ATOM	373	N	ASP	A	865	78.090	68.727	0.620	1.00	20.00
ATOM	374	CA	ASP	A	865	78.709	69.760	1.436	1.00	20.00
ATOM	375	C	ASP	A	865	78.128	69.958	2.819	1.00	20.00
ATOM	376	O	ASP	A	865	78.844	70.418	3.695	1.00	20.00
ATOM	377	CB	ASP	A	865	78.665	71.087	0.683	1.00	20.00
ATOM	379	N	HIS	A	866	76.832	69.683	3.014	1.00	20.00
ATOM	380	CA	HIS	A	866	76.223	69.807	4.364	1.00	20.00
ATOM	381	C	HIS	A	866	76.425	68.436	4.955	1.00	20.00
ATOM	382	O	HIS	A	866	76.537	68.227	6.178	1.00	20.00
ATOM	383	CB	HIS	A	866	74.699	70.145	4.303	1.00	20.00
ATOM	384	CG	HIS	A	866	73.836	69.068	3.706	1.00	20.00
ATOM	385	ND1	HIS	A	866	73.511	69.036	2.360	1.00	20.00
ATOM	386	CD2	HIS	A	866	73.145	68.054	4.285	1.00	20.00
ATOM	387	CE1	HIS	A	866	72.653	68.054	2.140	1.00	20.00
ATOM	388	NE2	HIS	A	866	72.416	67.443	3.290	1.00	20.00
ATOM	392	N	ARG	A	867	76.481	67.523	3.992	1.00	20.00
ATOM	393	CA	ARG	A	867	76.682	66.101	4.167	1.00	20.00
ATOM	394	C	ARG	A	867	77.752	65.727	5.193	1.00	20.00
ATOM	395	O	ARG	A	867	78.957	65.919	4.933	1.00	20.00
ATOM	396	CB	ARG	A	867	77.059	65.491	2.804	1.00	20.00
ATOM	397	CG	ARG	A	867	78.073	66.314	2.001	1.00	20.00
ATOM	398	CD	ARG	A	867	79.548	66.134	2.438	1.00	20.00
ATOM	399	NE	ARG	A	867	80.417	67.048	1.682	1.00	20.00
ATOM	400	CZ	ARG	A	867	81.270	67.924	2.231	1.00	20.00
ATOM	401	NH1	ARG	A	867	81.391	68.025	3.566	1.00	20.00
ATOM	402	NH2	ARG	A	867	81.977	68.729	1.428	1.00	20.00
ATOM	409	N	ASP	A	868	77.304	65.205	6.345	1.00	20.00
ATOM	410	CA	ASP	A	868	78.197	64.729	7.417	1.00	20.00
ATOM	411	C	ASP	A	868	77.784	63.290	7.881	1.00	20.00
ATOM	412	O	ASP	A	868	77.720	62.981	9.089	1.00	20.00
ATOM	413	CB	ASP	A	868	78.199	65.733	8.593	1.00	20.00
ATOM	414	CG	ASP	A	868	77.414	65.248	9.815	1.00	20.00
ATOM	415	OD1	ASP	A	868	76.266	64.747	9.611	1.00	20.00
ATOM	416	OD2	ASP	A	868	77.931	65.385	10.971	1.00	20.00
ATOM	418	N	PHE	A	869	77.560	62.391	6.921	1.00	20.00
ATOM	419	CA	PHE	A	869	77.119	61.033	7.261	1.00	20.00
ATOM	420	C	PHE	A	869	78.080	59.895	6.841	1.00	20.00
ATOM	421	O	PHE	A	869	78.526	59.819	5.663	1.00	20.00
ATOM	422	CB	PHE	A	869	75.738	60.806	6.625	1.00	20.00

FIG. 4F

ATOM	423	CG	PHE	A	869	75.685	61.221	5.199	1.00	20.00
ATOM	424	CD1	PHE	A	869	75.561	62.560	4.861	1.00	20.00
ATOM	425	CD2	PHE	A	869	75.848	60.286	4.190	1.00	20.00
ATOM	426	CE1	PHE	A	869	75.612	62.955	3.509	1.00	20.00
ATOM	427	CE2	PHE	A	869	75.896	60.680	2.838	1.00	20.00
ATOM	428	CZ	PHE	A	869	75.779	62.022	2.496	1.00	20.00
ATOM	430	N	ALA	A	870	78.350	59.018	7.812	1.00	20.00
ATOM	431	CA	ALA	A	870	79.231	57.831	7.715	1.00	20.00
ATOM	432	C	ALA	A	870	79.352	57.560	9.172	1.00	20.00
ATOM	433	O	ALA	A	870	78.350	57.359	9.840	1.00	20.00
ATOM	434	CB	ALA	A	870	80.624	58.132	7.160	1.00	20.00
ATOM	436	N	GLY	A	871	80.558	57.601	9.698	1.00	20.00
ATOM	437	CA	GLY	A	871	80.674	57.344	11.112	1.00	20.00
ATOM	438	C	GLY	A	871	79.343	57.592	11.791	1.00	20.00
ATOM	439	O	GLY	A	871	78.672	56.648	12.170	1.00	20.00
ATOM	441	N	GLU	A	872	78.958	58.864	11.901	1.00	20.00
ATOM	442	CA	GLU	A	872	77.690	59.258	12.529	1.00	20.00
ATOM	443	C	GLU	A	872	76.698	58.115	12.297	1.00	20.00
ATOM	444	O	GLU	A	872	76.096	57.579	13.241	1.00	20.00
ATOM	445	CB	GLU	A	872	77.178	60.602	11.939	1.00	20.00
ATOM	446	CG	GLU	A	872	76.581	60.552	10.530	1.00	20.00
ATOM	447	CD	GLU	A	872	75.027	60.750	10.507	1.00	20.00
ATOM	448	OE1	GLU	A	872	74.433	60.770	9.383	1.00	20.00
ATOM	449	OE2	GLU	A	872	74.405	60.881	11.596	1.00	20.00
ATOM	451	N	LEU	A	873	76.545	57.753	11.028	1.00	20.00
ATOM	452	CA	LEU	A	873	75.726	56.633	10.649	1.00	20.00
ATOM	453	C	LEU	A	873	76.593	55.505	11.273	1.00	20.00
ATOM	454	O	LEU	A	873	76.715	55.463	12.500	1.00	20.00
ATOM	455	CB	LEU	A	873	75.658	56.527	9.101	1.00	20.00
ATOM	457	N	GLU	A	874	77.195	54.620	10.458	1.00	20.00
ATOM	458	CA	GLU	A	874	78.069	53.539	10.975	1.00	20.00
ATOM	459	C	GLU	A	874	77.903	53.535	12.468	1.00	20.00
ATOM	460	O	GLU	A	874	76.948	52.968	12.998	1.00	20.00
ATOM	461	CB	GLU	A	874	79.526	53.831	10.639	1.00	20.00
ATOM	463	N	VAL	A	875	78.838	54.222	13.116	1.00	20.00
ATOM	464	CA	VAL	A	875	78.847	54.419	14.567	1.00	20.00
ATOM	465	C	VAL	A	875	77.770	53.658	15.342	1.00	20.00
ATOM	466	O	VAL	A	875	78.065	52.892	16.266	1.00	20.00
ATOM	467	CB	VAL	A	875	78.756	55.961	14.897	1.00	20.00
ATOM	469	N	LEU	A	876	76.520	53.887	14.966	1.00	20.00
ATOM	470	CA	LEU	A	876	75.408	53.237	15.630	1.00	20.00
ATOM	471	C	LEU	A	876	75.957	51.873	16.004	1.00	20.00
ATOM	472	O	LEU	A	876	75.727	51.387	17.126	1.00	20.00
ATOM	473	CB	LEU	A	876	74.208	53.192	14.684	1.00	20.00
ATOM	474	CG	LEU	A	876	73.839	54.662	14.399	1.00	20.00
ATOM	475	CD1	LEU	A	876	73.193	54.792	13.056	1.00	20.00
ATOM	476	CD2	LEU	A	876	72.942	55.198	15.481	1.00	20.00
ATOM	478	N	CYS	A	877	76.744	51.320	15.071	1.00	20.00
ATOM	479	CA	CYS	A	877	77.459	50.027	15.212	1.00	20.00
ATOM	480	C	CYS	A	877	77.658	49.645	16.685	1.00	20.00
ATOM	481	O	CYS	A	877	77.099	48.656	17.205	1.00	20.00
ATOM	482	CB	CYS	A	877	78.855	50.137	14.546	1.00	20.00
ATOM	483	SG	CYS	A	877	79.630	51.894	14.438	1.00	20.00
ATOM	485	N	LYS	A	878	78.447	50.496	17.337	1.00	20.00
ATOM	486	CA	LYS	A	878	78.789	50.363	18.762	1.00	20.00
ATOM	487	C	LYS	A	878	77.629	49.811	19.612	1.00	20.00
ATOM	488	O	LYS	A	878	77.847	49.438	20.805	1.00	20.00

FIG. 4G

ATOM	489	CB	LYS	A	878	79.260	51.733	19.351	1.00	20.00
ATOM	490	CG	LYS	A	878	80.718	52.114	19.017	1.00	20.00
ATOM	491	CD	LYS	A	878	81.321	52.986	20.114	1.00	20.00
ATOM	492	CE	LYS	A	878	81.612	54.418	19.609	1.00	20.00
ATOM	493	NZ	LYS	A	878	81.754	54.601	18.098	1.00	20.00
ATOM	498	N	LEU	A	879	76.427	49.792	19.000	1.00	20.00
ATOM	499	CA	LEU	A	879	75.203	49.320	19.634	1.00	20.00
ATOM	500	C	LEU	A	879	74.179	49.039	18.584	1.00	20.00
ATOM	501	O	LEU	A	879	73.068	49.544	18.652	1.00	20.00
ATOM	502	CB	LEU	A	879	74.620	50.336	20.651	1.00	20.00
ATOM	503	CG	LEU	A	879	74.799	51.863	20.603	1.00	20.00
ATOM	504	CD1	LEU	A	879	75.966	52.280	21.461	1.00	20.00
ATOM	505	CD2	LEU	A	879	75.015	52.321	19.200	1.00	20.00
ATOM	507	N	GLY	A	880	74.546	48.227	17.597	1.00	20.00
ATOM	508	CA	GLY	A	880	73.551	47.899	16.578	1.00	20.00
ATOM	509	C	GLY	A	880	72.345	47.314	17.330	1.00	20.00
ATOM	510	O	GLY	A	880	71.296	47.906	17.464	1.00	20.00
ATOM	512	N	HIS	A	881	72.545	46.101	17.820	1.00	20.00
ATOM	513	CA	HIS	A	881	71.575	45.353	18.572	1.00	20.00
ATOM	514	C	HIS	A	881	71.402	46.024	19.917	1.00	20.00
ATOM	515	O	HIS	A	881	71.758	47.183	20.106	1.00	20.00
ATOM	516	CB	HIS	A	881	72.059	43.906	18.744	1.00	20.00
ATOM	517	CG	HIS	A	881	71.015	42.958	19.255	1.00	20.00
ATOM	518	ND1	HIS	A	881	69.952	42.520	18.485	1.00	20.00
ATOM	519	CD2	HIS	A	881	70.877	42.349	20.464	1.00	20.00
ATOM	520	CE1	HIS	A	881	69.207	41.691	19.197	1.00	20.00
ATOM	521	NE2	HIS	A	881	69.746	41.566	20.402	1.00	20.00
ATOM	525	N	HIS	A	882	70.870	45.217	20.817	1.00	20.00
ATOM	526	CA	HIS	A	882	70.420	45.429	22.177	1.00	20.00
ATOM	527	C	HIS	A	882	68.935	45.241	21.763	1.00	20.00
ATOM	528	O	HIS	A	882	68.440	45.758	20.724	1.00	20.00
ATOM	529	CB	HIS	A	882	70.704	46.804	22.806	1.00	20.00
ATOM	530	CG	HIS	A	882	70.491	46.812	24.295	1.00	20.00
ATOM	531	ND1	HIS	A	882	69.252	46.654	24.868	1.00	20.00
ATOM	532	CD2	HIS	A	882	71.365	46.839	25.325	1.00	20.00
ATOM	533	CE1	HIS	A	882	69.373	46.579	26.183	1.00	20.00
ATOM	534	NE2	HIS	A	882	70.645	46.686	26.486	1.00	20.00
ATOM	538	N	PRO	A	883	68.210	44.463	22.547	1.00	20.00
ATOM	539	CA	PRO	A	883	66.820	44.253	22.152	1.00	20.00
ATOM	540	C	PRO	A	883	66.019	45.510	22.212	1.00	20.00
ATOM	541	O	PRO	A	883	65.100	45.685	21.439	1.00	20.00
ATOM	542	CB	PRO	A	883	66.309	43.176	23.108	1.00	20.00
ATOM	543	CG	PRO	A	883	67.285	43.129	24.211	1.00	20.00
ATOM	544	CD	PRO	A	883	68.560	43.829	23.819	1.00	20.00
ATOM	545	N	ASN	A	884	66.414	46.408	23.098	1.00	20.00
ATOM	546	CA	ASN	A	884	65.710	47.650	23.263	1.00	20.00
ATOM	547	C	ASN	A	884	66.169	48.856	22.439	1.00	20.00
ATOM	548	O	ASN	A	884	65.801	49.977	22.723	1.00	20.00
ATOM	549	CB	ASN	A	884	65.672	47.898	24.749	1.00	20.00
ATOM	550	CG	ASN	A	884	65.444	46.594	25.498	1.00	20.00
ATOM	551	OD1	ASN	A	884	65.835	46.388	26.649	1.00	20.00
ATOM	552	ND2	ASN	A	884	64.817	45.687	24.802	1.00	20.00
ATOM	556	N	ILE	A	885	66.917	48.603	21.375	1.00	20.00
ATOM	557	CA	ILE	A	885	67.391	49.655	20.482	1.00	20.00
ATOM	558	C	ILE	A	885	67.205	49.202	19.020	1.00	20.00
ATOM	559	O	ILE	A	885	67.847	48.251	18.589	1.00	20.00
ATOM	560	CB	ILE	A	885	68.930	50.021	20.761	1.00	20.00

FIG. 4H

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ATOM	561	CG1	ILE	A	885	69.032	50.962	21.954	1.00	20.00
ATOM	562	CG2	ILE	A	885	69.529	50.830	19.639	1.00	20.00
ATOM	563	CD1	ILE	A	885	70.397	51.213	22.385	1.00	20.00
ATOM	565	N	ILE	A	886	66.325	49.886	18.282	1.00	20.00
ATOM	566	CA	ILE	A	886	66.030	49.608	16.871	1.00	20.00
ATOM	567	C	ILE	A	886	67.338	49.271	16.206	1.00	20.00
ATOM	568	O	ILE	A	886	68.363	49.491	16.788	1.00	20.00
ATOM	569	CB	ILE	A	886	65.331	50.854	16.183	1.00	20.00
ATOM	570	CG1	ILE	A	886	63.806	50.758	16.349	1.00	20.00
ATOM	571	CG2	ILE	A	886	65.568	50.868	14.691	1.00	20.00
ATOM	572	CD1	ILE	A	886	63.134	49.624	15.492	1.00	20.00
ATOM	574	N	ASN	A	887	67.347	48.757	14.990	1.00	20.00
ATOM	575	CA	ASN	A	887	68.628	48.381	14.442	1.00	20.00
ATOM	576	C	ASN	A	887	68.846	48.692	13.013	1.00	20.00
ATOM	577	O	ASN	A	887	67.889	48.902	12.273	1.00	20.00
ATOM	578	CB	ASN	A	887	68.827	46.892	14.597	1.00	20.00
ATOM	579	CG	ASN	A	887	70.276	46.512	14.731	1.00	20.00
ATOM	580	OD1	ASN	A	887	71.015	46.382	13.725	1.00	20.00
ATOM	581	ND2	ASN	A	887	70.702	46.315	15.979	1.00	20.00
ATOM	585	N	LEU	A	888	70.118	48.684	12.604	1.00	20.00
ATOM	586	CA	LEU	A	888	70.417	48.950	11.203	1.00	20.00
ATOM	587	C	LEU	A	888	70.410	47.641	10.469	1.00	20.00
ATOM	588	O	LEU	A	888	71.128	46.705	10.852	1.00	20.00
ATOM	589	CB	LEU	A	888	71.799	49.586	11.000	1.00	20.00
ATOM	590	CG	LEU	A	888	72.125	49.333	9.517	1.00	20.00
ATOM	591	CD1	LEU	A	888	71.290	50.292	8.712	1.00	20.00
ATOM	592	CD2	LEU	A	888	73.594	49.451	9.207	1.00	20.00
ATOM	594	N	LEU	A	889	69.617	47.531	9.425	1.00	20.00
ATOM	595	CA	LEU	A	889	69.676	46.284	8.712	1.00	20.00
ATOM	596	C	LEU	A	889	70.630	46.494	7.567	1.00	20.00
ATOM	597	O	LEU	A	889	71.830	46.369	7.746	1.00	20.00
ATOM	598	CB	LEU	A	889	68.310	45.906	8.247	1.00	20.00
ATOM	599	CG	LEU	A	889	67.451	45.554	9.465	1.00	20.00
ATOM	600	CD1	LEU	A	889	66.321	44.719	8.913	1.00	20.00
ATOM	601	CD2	LEU	A	889	68.201	44.811	10.568	1.00	20.00
ATOM	603	N	GLY	A	890	70.114	46.838	6.396	1.00	20.00
ATOM	604	CA	GLY	A	890	70.971	47.127	5.254	1.00	20.00
ATOM	605	C	GLY	A	890	71.310	48.613	5.048	1.00	20.00
ATOM	606	O	GLY	A	890	71.237	49.441	5.951	1.00	20.00
ATOM	608	N	ALA	A	891	71.684	48.930	3.819	1.00	20.00
ATOM	609	CA	ALA	A	891	72.084	50.262	3.393	1.00	20.00
ATOM	610	C	ALA	A	891	72.437	50.082	1.907	1.00	20.00
ATOM	611	O*	ALA	A	891	72.299	48.965	1.361	1.00	20.00
ATOM	612	CB	ALA	A	891	73.296	50.706	4.166	1.00	20.00
ATOM	614	N	CYS	A	892	72.908	51.153	1.262	1.00	20.00
ATOM	615	CA	CYS	A	892	73.258	51.085	-0.166	1.00	20.00
ATOM	616	C	CYS	A	892	73.174	52.468	-0.776	1.00	20.00
ATOM	617	O	CYS	A	892	72.263	53.232	-0.453	1.00	20.00
ATOM	618	CB	CYS	A	892	72.277	50.171	-0.952	1.00	20.00
ATOM	619	SG	CYS	A	892	72.953	48.465	-1.345	1.00	20.00
ATOM	621	N	GLU	A	893	74.089	52.785	-1.680	1.00	20.00
ATOM	622	CA	GLU	A	893	74.062	54.101	-2.298	1.00	20.00
ATOM	623	C	GLU	A	893	73.386	54.004	-3.637	1.00	20.00
ATOM	624	O	GLU	A	893	73.956	53.509	-4.616	1.00	20.00
ATOM	625	CB	GLU	A	893	75.483	54.655	-2.463	1.00	20.00
ATOM	626	CG	GLU	A	893	76.613	53.751	-1.900	1.00	20.00
ATOM	627	CD	GLU	A	893	77.227	52.860	-2.966	1.00	20.00

FIG. 4I

ATOM	628	OE1	GLU	A	893	76.831	52.998	-4.151	1.00	20.00
ATOM	629	OE2	GLU	A	893	78.105	52.033	-2.612	1.00	20.00
ATOM	631	N	HIS	A	894	72.140	54.427	-3.684	1.00	20.00
ATOM	632	CA	HIS	A	894	71.437	54.382	-4.949	1.00	20.00
ATOM	633	C	HIS	A	894	71.690	55.786	-5.419	1.00	20.00
ATOM	634	O	HIS	A	894	71.305	56.755	-4.750	1.00	20.00
ATOM	635	CB	HIS	A	894	69.937	54.149	-4.753	1.00	20.00
ATOM	636	CG	HIS	A	894	69.133	54.328	-6.003	1.00	20.00
ATOM	637	ND1	HIS	A	894	67.767	54.494	-5.990	1.00	20.00
ATOM	638	CD2	HIS	A	894	69.510	54.413	-7.301	1.00	20.00
ATOM	639	CE1	HIS	A	894	67.332	54.680	-7.223	1.00	20.00
ATOM	640	NE2	HIS	A	894	68.369	54.634	-8.037	1.00	20.00
ATOM	644	N	ARG	A	895	72.366	55.873	-6.556	1.00	20.00
ATOM	645	CA	ARG	A	895	72.768	57.132	-7.151	1.00	20.00
ATOM	646	C	ARG	A	895	71.873	58.311	-6.767	1.00	20.00
ATOM	647	O	ARG	A	895	70.654	58.317	-7.001	1.00	20.00
ATOM	648	CB	ARG	A	895	72.910	56.904	-8.643	1.00	20.00
ATOM	649	CG	ARG	A	895	73.918	55.775	-8.856	1.00	20.00
ATOM	650	CD	ARG	A	895	73.482	54.825	-9.910	1.00	20.00
ATOM	651	NE	ARG	A	895	74.001	55.309	-11.176	1.00	20.00
ATOM	652	CZ	ARG	A	895	73.609	54.881	-12.370	1.00	20.00
ATOM	653	NH1	ARG	A	895	72.657	53.926	-12.469	1.00	20.00
ATOM	654	NH2	ARG	A	895	74.183	55.416	-13.460	1.00	20.00
ATOM	661	N	GLY	A	896	72.510	59.315	-6.177	1.00	20.00
ATOM	662	CA	GLY	A	896	71.781	60.441	-5.654	1.00	20.00
ATOM	663	C	GLY	A	896	71.963	60.040	-4.207	1.00	20.00
ATOM	664	O	GLY	A	896	72.194	58.860	-3.967	1.00	20.00
ATOM	666	N	TYR	A	897	71.919	60.962	-3.254	1.00	20.00
ATOM	667	CA	TYR	A	897	72.066	60.604	-1.839	1.00	20.00
ATOM	668	C	TYR	A	897	71.643	59.133	-1.531	1.00	20.00
ATOM	669	O	TYR	A	897	70.959	58.507	-2.336	1.00	20.00
ATOM	670	CB	TYR	A	897	71.195	61.548	-1.039	1.00	20.00
ATOM	671	CG	TYR	A	897	71.828	62.224	0.128	1.00	20.00
ATOM	672	CD1	TYR	A	897	73.097	62.810	0.030	1.00	20.00
ATOM	673	CD2	TYR	A	897	71.116	62.358	1.321	1.00	20.00
ATOM	674	CE1	TYR	A	897	73.638	63.526	1.108	1.00	20.00
ATOM	675	CE2	TYR	A	897	71.641	63.069	2.402	1.00	20.00
ATOM	676	CZ	TYR	A	897	72.894	63.650	2.290	1.00	20.00
ATOM	677	OH	TYR	A	897	73.381	64.361	3.369	1.00	20.00
ATOM	680	N	LEU	A	898	72.001	58.564	-0.369	1.00	20.00
ATOM	681	CA	LEU	A	898	71.571	57.163	-0.196	1.00	20.00
ATOM	682	C	LEU	A	898	71.131	56.437	1.099	1.00	20.00
ATOM	683	O	LEU	A	898	71.759	56.483	2.161	1.00	20.00
ATOM	684	CB	LEU	A	898	72.542	56.240	-0.990	1.00	20.00
ATOM	686	N	TYR	A	899	70.041	55.704	0.830	1.00	20.00
ATOM	687	CA	TYR	A	899	69.162	54.833	1.624	1.00	20.00
ATOM	688	C	TYR	A	899	69.544	53.804	2.665	1.00	20.00
ATOM	689	O	TYR	A	899	70.411	52.969	2.445	1.00	20.00
ATOM	690	CB	TYR	A	899	68.268	54.076	0.657	1.00	20.00
ATOM	691	CG	TYR	A	899	67.523	54.943	-0.339	1.00	20.00
ATOM	692	CD1	TYR	A	899	68.208	55.776	-1.209	1.00	20.00
ATOM	693	CD2	TYR	A	899	66.163	54.790	-0.522	1.00	20.00
ATOM	694	CE1	TYR	A	899	67.574	56.407	-2.238	1.00	20.00
ATOM	695	CE2	TYR	A	899	65.514	55.429	-1.564	1.00	20.00
ATOM	696	CZ	TYR	A	899	66.225	56.235	-2.431	1.00	20.00
ATOM	697	OH	TYR	A	899	65.602	56.841	-3.510	1.00	20.00
ATOM	700	N	LEU	A	900	68.814	53.814	3.775	1.00	20.00

FIG. 4J

ATOM	701	CA	LEU	A	900	69.047	52.841	4.845	1.00	20.00
ATOM	702	C	LEU	A	900	67.805	51.988	5.149	1.00	20.00
ATOM	703	O	LEU	A	900	66.645	52.459	5.109	1.00	20.00
ATOM	704	CB	LEU	A	900	69.455	53.522	6.147	1.00	20.00
ATOM	705	CG	LEU	A	900	70.810	54.184	6.259	1.00	20.00
ATOM	706	CD1	LEU	A	900	71.404	54.368	4.864	1.00	20.00
ATOM	707	CD2	LEU	A	900	70.624	55.498	7.033	1.00	20.00
ATOM	709	N	ALA	A	901	68.083	50.739	5.495	1.00	20.00
ATOM	710	CA	ALA	A	901	67.043	49.813	5.811	1.00	20.00
ATOM	711	C	ALA	A	901	67.113	49.495	7.275	1.00	20.00
ATOM	712	O	ALA	A	901	67.828	48.577	7.670	1.00	20.00
ATOM	713	CB	ALA	A	901	67.221	48.564	5.003	1.00	20.00
ATOM	715	N	ILE	A	902	66.372	50.260	8.078	1.00	20.00
ATOM	716	CA	ILE	A	902	66.310	50.058	9.513	1.00	20.00
ATOM	717	C	ILE	A	902	65.367	48.888	9.812	1.00	20.00
ATOM	718	O	ILE	A	902	64.702	48.383	8.917	1.00	20.00
ATOM	719	CB	ILE	A	902	65.801	51.315	10.167	1.00	20.00
ATOM	720	CG1	ILE	A	902	66.882	52.398	10.058	1.00	20.00
ATOM	721	CG2	ILE	A	902	65.308	51.006	11.556	1.00	20.00
ATOM	722	CD1	ILE	A	902	67.878	52.583	11.280	1.00	20.00
ATOM	724	N	GLU	A	903	65.322	48.439	11.057	1.00	20.00
ATOM	725	CA	GLU	A	903	64.435	47.350	11.465	1.00	20.00
ATOM	726	C	GLU	A	903	62.997	47.870	11.692	1.00	20.00
ATOM	727	O	GLU	A	903	62.713	48.559	12.662	1.00	20.00
ATOM	728	CB	GLU	A	903	64.973	46.703	12.746	1.00	20.00
ATOM	729	CG	GLU	A	903	63.985	45.965	13.580	1.00	20.00
ATOM	730	CD	GLU	A	903	64.471	45.766	15.006	1.00	20.00
ATOM	731	OE1	GLU	A	903	63.971	44.875	15.725	1.00	20.00
ATOM	732	OE2	GLU	A	903	65.365	46.509	15.425	1.00	20.00
ATOM	734	N	TYR	A	904	62.115	47.514	10.767	1.00	20.00
ATOM	735	CA	TYR	A	904	60.707	47.846	10.758	1.00	20.00
ATOM	736	C	TYR	A	904	59.985	47.328	11.989	1.00	20.00
ATOM	737	O	TYR	A	904	60.054	46.149	12.240	1.00	20.00
ATOM	738	CB	TYR	A	904	60.078	47.204	9.521	1.00	20.00
ATOM	739	CG	TYR	A	904	58.553	47.146	9.537	1.00	20.00
ATOM	740	CD1	TYR	A	904	57.795	48.150	8.920	1.00	20.00
ATOM	741	CD2	TYR	A	904	57.868	46.125	10.188	1.00	20.00
ATOM	742	CE1	TYR	A	904	56.420	48.136	8.955	1.00	20.00
ATOM	743	CE2	TYR	A	904	56.498	46.115	10.223	1.00	20.00
ATOM	744	CZ	TYR	A	904	55.779	47.128	9.602	1.00	20.00
ATOM	745	OH	TYR	A	904	54.405	47.149	9.622	1.00	20.00
ATOM	748	N	ALA	A	905	59.270	48.183	12.727	1.00	20.00
ATOM	749	CA	ALA	A	905	58.503	47.772	13.931	1.00	20.00
ATOM	750	C	ALA	A	905	56.987	47.506	13.620	1.00	20.00
ATOM	751	O	ALA	A	905	56.395	48.128	12.744	1.00	20.00
ATOM	752	CB	ALA	A	905	58.649	48.816	14.976	1.00	20.00
ATOM	754	N	PRO	A	906	56.341	46.572	14.317	1.00	20.00
ATOM	755	CA	PRO	A	906	54.949	46.394	13.918	1.00	20.00
ATOM	756	C	PRO	A	906	53.803	46.643	14.902	1.00	20.00
ATOM	757	O	PRO	A	906	52.992	45.748	15.150	1.00	20.00
ATOM	758	CB	PRO	A	906	54.958	44.937	13.468	1.00	20.00
ATOM	759	CG	PRO	A	906	55.981	44.280	14.584	1.00	20.00
ATOM	760	CD	PRO	A	906	56.719	45.482	15.227	1.00	20.00
ATOM	761	N	HIS	A	907	53.729	47.841	15.450	1.00	20.00
ATOM	762	CA	HIS	A	907	52.655	48.251	16.349	1.00	20.00
ATOM	763	C	HIS	A	907	52.966	49.700	16.468	1.00	20.00
ATOM	764	O	HIS	A	907	52.865	50.262	17.534	1.00	20.00

FIG. 4K

ATOM	765	CB	HIS	A	907	52.745	47.577	17.714	1.00	20.00
ATOM	766	CG	HIS	A	907	52.656	46.090	17.650	1.00	20.00
ATOM	767	ND1	HIS	A	907	53.753	45.272	17.799	1.00	20.00
ATOM	768	CD2	HIS	A	907	51.622	45.274	17.350	1.00	20.00
ATOM	769	CE1	HIS	A	907	53.404	44.018	17.593	1.00	20.00
ATOM	770	NE2	HIS	A	907	52.116	43.993	17.318	1.00	20.00
ATOM	774	N	GLY	A	908	53.411	50.280	15.365	1.00	20.00
ATOM	775	CA	GLY	A	908	53.733	51.676	15.348	1.00	20.00
ATOM	776	C	GLY	A	908	54.622	52.111	16.486	1.00	20.00
ATOM	777	O	GLY	A	908	55.525	51.381	16.887	1.00	20.00
ATOM	779	N	ASN	A	909	54.338	53.284	17.054	1.00	20.00
ATOM	780	CA	ASN	A	909	55.183	53.854	18.094	1.00	20.00
ATOM	781	C	ASN	A	909	54.590	53.912	19.463	1.00	20.00
ATOM	782	O	ASN	A	909	53.409	54.064	19.616	1.00	20.00
ATOM	783	CB	ASN	A	909	55.545	55.270	17.672	1.00	20.00
ATOM	784	CG	ASN	A	909	54.346	56.201	17.669	1.00	20.00
ATOM	785	OD1	ASN	A	909	54.409	57.315	17.192	1.00	20.00
ATOM	786	ND2	ASN	A	909	53.260	55.738	18.210	1.00	20.00
ATOM	790	N	LEU	A	910	55.414	53.878	20.482	1.00	20.00
ATOM	791	CA	LEU	A	910	54.872	53.913	21.808	1.00	20.00
ATOM	792	C	LEU	A	910	53.703	54.890	21.927	1.00	20.00
ATOM	793	O	LEU	A	910	52.760	54.647	22.669	1.00	20.00
ATOM	794	CB	LEU	A	910	55.949	54.257	22.797	1.00	20.00
ATOM	795	CG	LEU	A	910	55.456	54.079	24.220	1.00	20.00
ATOM	796	CD1	LEU	A	910	54.921	52.676	24.488	1.00	20.00
ATOM	797	CD2	LEU	A	910	56.617	54.427	25.133	1.00	20.00
ATOM	799	N	LEU	A	911	53.725	56.005	21.219	1.00	20.00
ATOM	800	CA	LEU	A	911	52.578	56.862	21.381	1.00	20.00
ATOM	801	C	LEU	A	911	51.408	56.200	20.656	1.00	20.00
ATOM	802	O	LEU	A	911	50.700	55.442	21.275	1.00	20.00
ATOM	803	CB	LEU	A	911	52.820	58.302	20.863	1.00	20.00
ATOM	804	CG	LEU	A	911	51.958	59.498	21.354	1.00	20.00
ATOM	805	CD1	LEU	A	911	51.738	59.517	22.855	1.00	20.00
ATOM	806	CD2	LEU	A	911	52.645	60.737	20.917	1.00	20.00
ATOM	808	N	ASP	A	912	51.219	56.459	19.371	1.00	20.00
ATOM	809	CA	ASP	A	912	50.117	55.895	18.642	1.00	20.00
ATOM	810	C	ASP	A	912	49.646	54.540	19.121	1.00	20.00
ATOM	811	O	ASP	A	912	48.468	54.225	19.083	1.00	20.00
ATOM	812	CB	ASP	A	912	50.461	55.849	17.181	1.00	20.00
ATOM	813	CG	ASP	A	912	50.214	57.151	16.498	1.00	20.00
ATOM	814	OD1	ASP	A	912	50.507	57.259	15.304	1.00	20.00
ATOM	815	OD2	ASP	A	912	49.725	58.089	17.141	1.00	20.00
ATOM	817	N	PHE	A	913	50.572	53.703	19.562	1.00	20.00
ATOM	818	CA	PHE	A	913	50.168	52.405	20.098	1.00	20.00
ATOM	819	C	PHE	A	913	49.397	52.903	21.287	1.00	20.00
ATOM	820	O	PHE	A	913	48.236	53.231	21.164	1.00	20.00
ATOM	821	CB	PHE	A	913	51.355	51.585	20.547	1.00	20.00
ATOM	822	CG	PHE	A	913	51.010	50.182	20.847	1.00	20.00
ATOM	823	CD1	PHE	A	913	50.511	49.365	19.866	1.00	20.00
ATOM	824	CD2	PHE	A	913	51.133	49.688	22.122	1.00	20.00
ATOM	825	CE1	PHE	A	913	50.141	48.088	20.152	1.00	20.00
ATOM	826	CE2	PHE	A	913	50.760	48.418	22.407	1.00	20.00
ATOM	827	CZ	PHE	A	913	50.263	47.619	21.418	1.00	20.00
ATOM	829	N	LEU	A	914	50.059	53.031	22.416	1.00	20.00
ATOM	830	CA	LEU	A	914	49.400	53.584	23.572	1.00	20.00
ATOM	831	C	LEU	A	914	48.080	54.304	23.288	1.00	20.00
ATOM	832	O	LEU	A	914	47.102	54.093	23.985	1.00	20.00

FIG. 4L

ATOM	833	CB	LEU	A	914	50.342	54.549	24.244	1.00	20.00
ATOM	834	CG	LEU	A	914	51.146	53.995	25.410	1.00	20.00
ATOM	835	CD1	LEU	A	914	52.130	55.080	25.953	1.00	20.00
ATOM	836	CD2	LEU	A	914	50.142	53.501	26.466	1.00	20.00
ATOM	838	N	ARG	A	915	48.006	55.139	22.265	1.00	20.00
ATOM	839	CA	ARG	A	915	46.736	55.841	22.041	1.00	20.00
ATOM	840	C	ARG	A	915	45.650	54.970	21.526	1.00	20.00
ATOM	841	O	ARG	A	915	44.569	54.984	22.054	1.00	20.00
ATOM	842	CB	ARG	A	915	46.896	57.078	21.141	1.00	20.00
ATOM	843	CG	ARG	A	915	46.687	58.379	21.885	1.00	20.00
ATOM	844	CD	ARG	A	915	47.528	59.415	21.256	1.00	20.00
ATOM	845	NE	ARG	A	915	48.215	60.347	22.169	1.00	20.00
ATOM	846	CZ	ARG	A	915	48.763	61.482	21.760	1.00	20.00
ATOM	847	NH1	ARG	A	915	48.709	61.835	20.494	1.00	20.00
ATOM	848	NH2	ARG	A	915	49.383	62.240	22.602	1.00	20.00
ATOM	855	N	LYS	A	916	45.943	54.219	20.485	1.00	20.00
ATOM	856	CA	LYS	A	916	45.019	53.242	19.890	1.00	20.00
ATOM	857	C	LYS	A	916	44.681	52.169	20.920	1.00	20.00
ATOM	858	O	LYS	A	916	44.275	51.109	20.561	1.00	20.00
ATOM	859	CB	LYS	A	916	45.714	52.563	18.676	1.00	20.00
ATOM	860	CG	LYS	A	916	45.988	51.000	18.704	1.00	20.00
ATOM	861	CD	LYS	A	916	46.802	50.408	19.888	1.00	20.00
ATOM	862	CE	LYS	A	916	46.861	48.841	19.822	1.00	20.00
ATOM	863	NZ	LYS	A	916	46.225	47.974	20.937	1.00	20.00
ATOM	868	N	SER	A	917	44.851	52.438	22.196	1.00	20.00
ATOM	869	CA	SER	A	917	44.597	51.466	23.204	1.00	20.00
ATOM	870	C	SER	A	917	43.641	52.011	24.233	1.00	20.00
ATOM	871	O	SER	A	917	43.501	51.444	25.330	1.00	20.00
ATOM	872	CB	SER	A	917	45.891	51.147	23.883	1.00	20.00
ATOM	873	OG	SER	A	917	45.843	51.568	25.227	1.00	20.00
ATOM	876	N	ARG	A	918	43.014	53.138	23.902	1.00	20.00
ATOM	877	CA	ARG	A	918	42.041	53.822	24.775	1.00	20.00
ATOM	878	C	ARG	A	918	40.816	53.359	24.014	1.00	20.00
ATOM	879	O	ARG	A	918	40.523	53.883	22.951	1.00	20.00
ATOM	880	CB	ARG	A	918	42.260	55.365	24.669	1.00	20.00
ATOM	881	CG	ARG	A	918	43.138	56.036	25.794	1.00	20.00
ATOM	882	CD	ARG	A	918	43.547	57.502	25.488	1.00	20.00
ATOM	883	NE	ARG	A	918	44.494	57.982	26.502	1.00	20.00
ATOM	884	CZ	ARG	A	918	44.777	59.260	26.795	1.00	20.00
ATOM	885	NH1	ARG	A	918	44.211	60.289	26.165	1.00	20.00
ATOM	886	NH2	ARG	A	918	45.625	59.523	27.777	1.00	20.00
ATOM	893	N	VAL	A	919	40.135	52.333	24.507	1.00	20.00
ATOM	894	CA	VAL	A	919	39.009	51.770	23.757	1.00	20.00
ATOM	895	C	VAL	A	919	37.733	52.382	24.202	1.00	20.00
ATOM	896	O	VAL	A	919	36.750	52.427	23.450	1.00	20.00
ATOM	897	CB	VAL	A	919	38.925	50.198	23.861	1.00	20.00
ATOM	898	CG1	VAL	A	919	40.218	49.603	23.459	1.00	20.00
ATOM	899	CG2	VAL	A	919	38.550	49.746	25.275	1.00	20.00
ATOM	901	N	LEU	A	920	37.736	52.861	25.432	1.00	20.00
ATOM	902	CA	LEU	A	920	36.569	53.542	25.895	1.00	20.00
ATOM	903	C	LEU	A	920	36.303	54.630	24.864	1.00	20.00
ATOM	904	O	LEU	A	920	35.276	55.259	24.906	1.00	20.00
ATOM	905	CB	LEU	A	920	36.815	54.146	27.236	1.00	20.00
ATOM	906	CG	LEU	A	920	35.641	54.652	28.011	1.00	20.00
ATOM	907	CD1	LEU	A	920	35.060	53.567	28.831	1.00	20.00
ATOM	908	CD2	LEU	A	920	36.155	55.768	28.901	1.00	20.00
ATOM	910	N	GLU	A	921	37.224	54.824	23.926	1.00	20.00

FIG. 4M

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ATOM	911	CA	GLU	A	921	37.081	55.783	22.850	1.00	20.00
ATOM	912	C	GLU	A	921	37.413	55.109	21.541	1.00	20.00
ATOM	913	O	GLU	A	921	37.205	55.677	20.469	1.00	20.00
ATOM	914	CB	GLU	A	921	38.047	56.940	23.011	1.00	20.00
ATOM	915	CG	GLU	A	921	38.258	57.743	21.736	1.00	20.00
ATOM	916	CD	GLU	A	921	39.404	58.696	21.848	1.00	20.00
ATOM	917	OE1	GLU	A	921	39.875	58.879	22.982	1.00	20.00
ATOM	918	OE2	GLU	A	921	39.836	59.261	20.825	1.00	20.00
ATOM	920	N	THR	A	922	37.936	53.893	21.615	1.00	20.00
ATOM	921	CA	THR	A	922	38.309	53.178	20.413	1.00	20.00
ATOM	922	C	THR	A	922	37.429	51.960	20.078	1.00	20.00
ATOM	923	O	THR	A	922	37.502	51.387	18.963	1.00	20.00
ATOM	924	CB	THR	A	922	39.742	52.728	20.559	1.00	20.00
ATOM	925	OG1	THR	A	922	40.441	53.058	19.366	1.00	20.00
ATOM	926	CG2	THR	A	922	39.824	51.214	20.816	1.00	20.00
ATOM	929	N	ASP	A	923	36.617	51.575	21.074	1.00	20.00
ATOM	930	CA	ASP	A	923	35.712	50.423	21.026	1.00	20.00
ATOM	931	C	ASP	A	923	34.972	50.387	22.350	1.00	20.00
ATOM	932	O	ASP	A	923	35.259	49.550	23.203	1.00	20.00
ATOM	933	CB	ASP	A	923	36.494	49.119	20.905	1.00	20.00
ATOM	934	CG	ASP	A	923	35.879	48.142	19.909	1.00	20.00
ATOM	935	OD1	ASP	A	923	35.624	48.553	18.745	1.00	20.00
ATOM	936	OD2	ASP	A	923	35.669	46.956	20.271	1.00	20.00
ATOM	938	N	PRO	A	924	34.042	51.323	22.577	1.00	20.00
ATOM	939	CA	PRO	A	924	33.362	51.211	23.874	1.00	20.00
ATOM	940	C	PRO	A	924	32.544	49.923	24.176	1.00	20.00
ATOM	941	O	PRO	A	924	32.172	49.720	25.342	1.00	20.00
ATOM	942	CB	PRO	A	924	32.540	52.506	23.953	1.00	20.00
ATOM	943	CG	PRO	A	924	33.214	53.417	22.960	1.00	20.00
ATOM	944	CD	PRO	A	924	33.600	52.512	21.841	1.00	20.00
ATOM	945	N	ALA	A	925	32.276	49.078	23.156	1.00	20.00
ATOM	946	CA	ALA	A	925	31.551	47.770	23.326	1.00	20.00
ATOM	947	C	ALA	A	925	32.438	46.878	24.193	1.00	20.00
ATOM	948	O	ALA	A	925	32.016	46.274	25.190	1.00	20.00
ATOM	949	CB	ALA	A	925	31.328	47.103	21.992	1.00	20.00
ATOM	951	N	PHE	A	926	33.695	46.843	23.771	1.00	20.00
ATOM	952	CA	PHE	A	926	34.782	46.173	24.431	1.00	20.00
ATOM	953	C	PHE	A	926	34.885	46.856	25.745	1.00	20.00
ATOM	954	O	PHE	A	926	34.896	46.269	26.772	1.00	20.00
ATOM	955	CB	PHE	A	926	36.058	46.460	23.667	1.00	20.00
ATOM	956	CG	PHE	A	926	37.046	45.347	23.693	1.00	20.00
ATOM	957	CD1	PHE	A	926	37.164	44.511	22.599	1.00	20.00
ATOM	958	CD2	PHE	A	926	37.810	45.127	24.825	1.00	20.00
ATOM	959	CE1	PHE	A	926	38.003	43.493	22.630	1.00	20.00
ATOM	960	CE2	PHE	A	926	38.661	44.107	24.881	1.00	20.00
ATOM	961	CZ	PHE	A	926	38.773	43.272	23.786	1.00	20.00
ATOM	963	N	ALA	A	927	35.024	48.154	25.681	1.00	20.00
ATOM	964	CA	ALA	A	927	35.084	48.926	26.885	1.00	20.00
ATOM	965	C	ALA	A	927	34.165	48.337	27.956	1.00	20.00
ATOM	966	O	ALA	A	927	34.695	47.721	28.843	1.00	20.00
ATOM	967	CB	ALA	A	927	34.717	50.348	26.587	1.00	20.00
ATOM	969	N	ILE	A	928	32.825	48.502	27.887	1.00	20.00
ATOM	970	CA	ILE	A	928	31.935	47.945	28.958	1.00	20.00
ATOM	971	C	ILE	A	928	31.760	46.437	29.001	1.00	20.00
ATOM	972	O	ILE	A	928	31.464	45.883	30.050	1.00	20.00
ATOM	973	CB	ILE	A	928	30.395	48.487	29.019	1.00	20.00
ATOM	974	CG1	ILE	A	928	30.081	49.486	27.941	1.00	20.00

FIG. 4N

ATOM	975	CG2	ILE	A	928	30.098	49.114	30.414	1.00	20.00
ATOM	976	CD1	ILE	A	928	29.952	50.862	28.545	1.00	20.00
ATOM	978	N	ALA	A	929	31.895	45.782	27.860	1.00	20.00
ATOM	979	CA	ALA	A	929	31.747	44.356	27.867	1.00	20.00
ATOM	980	C	ALA	A	929	32.803	43.844	28.804	1.00	20.00
ATOM	981	O	ALA	A	929	32.525	43.055	29.667	1.00	20.00
ATOM	982	CB	ALA	A	929	31.946	43.823	26.510	1.00	20.00
ATOM	984	N	ASN	A	930	34.010	44.358	28.642	1.00	20.00
ATOM	985	CA	ASN	A	930	35.181	44.009	29.429	1.00	20.00
ATOM	986	C	ASN	A	930	35.448	44.882	30.665	1.00	20.00
ATOM	987	O	ASN	A	930	36.191	44.496	31.566	1.00	20.00
ATOM	988	CB	ASN	A	930	36.397	44.067	28.511	1.00	20.00
ATOM	989	CG	ASN	A	930	36.628	42.771	27.745	1.00	20.00
ATOM	990	OD1	ASN	A	930	37.333	41.876	28.220	1.00	20.00
ATOM	991	ND2	ASN	A	930	36.046	42.671	26.547	1.00	20.00
ATOM	995	N	SER	A	931	34.847	46.063	30.695	1.00	20.00
ATOM	996	CA	SER	A	931	35.050	47.041	31.768	1.00	20.00
ATOM	997	C	SER	A	931	36.531	47.527	31.922	1.00	20.00
ATOM	998	O	SER	A	931	37.074	47.556	33.020	1.00	20.00
ATOM	999	CB	SER	A	931	34.541	46.453	33.084	1.00	20.00
ATOM	1000	OG	SER	A	931	34.196	45.103	32.879	1.00	20.00
ATOM	1003	N	THR	A	932	37.155	47.931	30.815	1.00	20.00
ATOM	1004	CA	THR	A	932	38.545	48.392	30.821	1.00	20.00
ATOM	1005	C	THR	A	932	38.800	49.536	29.872	1.00	20.00
ATOM	1006	O	THR	A	932	38.184	49.614	28.803	1.00	20.00
ATOM	1007	CB	THR	A	932	39.525	47.299	30.451	1.00	20.00
ATOM	1008	OG1	THR	A	932	38.971	46.481	29.417	1.00	20.00
ATOM	1009	CG2	THR	A	932	39.832	46.479	31.663	1.00	20.00
ATOM	1012	N	ALA	A	933	39.747	50.384	30.287	1.00	20.00
ATOM	1013	CA	ALA	A	933	40.179	51.608	29.597	1.00	20.00
ATOM	1014	C	ALA	A	933	41.172	51.417	28.495	1.00	20.00
ATOM	1015	O	ALA	A	933	41.155	52.134	27.513	1.00	20.00
ATOM	1016	CB	ALA	A	933	40.778	52.547	30.597	1.00	20.00
ATOM	1018	N	SER	A	934	42.086	50.480	28.709	1.00	20.00
ATOM	1019	CA	SER	A	934	43.134	50.131	27.749	1.00	20.00
ATOM	1020	C	SER	A	934	43.001	48.645	27.512	1.00	20.00
ATOM	1021	O	SER	A	934	42.431	47.966	28.337	1.00	20.00
ATOM	1022	CB	SER	A	934	44.511	50.396	28.374	1.00	20.00
ATOM	1023	OG	SER	A	934	45.494	50.638	27.386	1.00	20.00
ATOM	1026	N	THR	A	935	43.497	48.150	26.380	1.00	20.00
ATOM	1027	CA	THR	A	935	43.529	46.701	26.144	1.00	20.00
ATOM	1028	C	THR	A	935	44.801	46.297	26.814	1.00	20.00
ATOM	1029	O	THR	A	935	45.015	45.118	27.082	1.00	20.00
ATOM	1030	CB	THR	A	935	43.768	46.312	24.783	1.00	20.00
ATOM	1031	OG1	THR	A	935	44.892	47.021	24.325	1.00	20.00
ATOM	1032	CG2	THR	A	935	42.571	46.583	23.961	1.00	20.00
ATOM	1035	N	LEU	A	936	45.640	47.301	27.070	1.00	20.00
ATOM	1036	CA	LEU	A	936	46.897	47.138	27.735	1.00	20.00
ATOM	1037	C	LEU	A	936	46.640	46.822	29.174	1.00	20.00
ATOM	1038	O	LEU	A	936	45.579	47.010	29.666	1.00	20.00
ATOM	1039	CB	LEU	A	936	47.699	48.413	27.635	1.00	20.00
ATOM	1040	CG	LEU	A	936	47.921	49.086	26.273	1.00	20.00
ATOM	1041	CD1	LEU	A	936	49.058	50.134	26.370	1.00	20.00
ATOM	1042	CD2	LEU	A	936	48.250	48.029	25.238	1.00	20.00
ATOM	1044	N	SER	A	937	47.652	46.322	29.841	1.00	20.00
ATOM	1045	CA	SER	A	937	47.576	45.961	31.232	1.00	20.00
ATOM	1046	C	SER	A	937	48.521	46.834	32.054	1.00	20.00

FIG. 40

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ATOM	1047	O	SER A 937	49.291	47.608	31.519	1.00	20.00
ATOM	1048	CB	SER A 937	47.988	44.501	31.384	1.00	20.00
ATOM	1049	OG	SER A 937	48.630	44.257	32.628	1.00	20.00
ATOM	1052	N	SER A 938	48.458	46.695	33.365	1.00	20.00
ATOM	1053	CA	SER A 938	49.319	47.433	34.239	1.00	20.00
ATOM	1054	C	SER A 938	50.724	46.904	33.957	1.00	20.00
ATOM	1055	O	SER A 938	51.686	47.668	33.847	1.00	20.00
ATOM	1056	CB	SER A 938	48.900	47.177	35.683	1.00	20.00
ATOM	1057	OG	SER A 938	50.012	47.071	36.555	1.00	20.00
ATOM	1060	N	GLN A 939	50.849	45.587	33.812	1.00	20.00
ATOM	1061	CA	GLN A 939	52.165	45.002	33.522	1.00	20.00
ATOM	1062	C	GLN A 939	52.709	45.435	32.165	1.00	20.00
ATOM	1063	O	GLN A 939	53.831	45.917	32.073	1.00	20.00
ATOM	1064	CB	GLN A 939	52.138	43.465	33.608	1.00	20.00
ATOM	1065	CG	GLN A 939	52.298	42.909	35.046	1.00	20.00
ATOM	1066	CD	GLN A 939	53.756	42.716	35.473	1.00	20.00
ATOM	1067	OE1	GLN A 939	54.595	42.185	34.711	1.00	20.00
ATOM	1068	NE2	GLN A 939	54.065	43.139	36.700	1.00	20.00
ATOM	1072	N	GLN A 940	51.932	45.294	31.111	1.00	20.00
ATOM	1073	CA	GLN A 940	52.445	45.696	29.813	1.00	20.00
ATOM	1074	C	GLN A 940	53.040	47.092	29.913	1.00	20.00
ATOM	1075	O	GLN A 940	53.944	47.477	29.163	1.00	20.00
ATOM	1076	CB	GLN A 940	51.330	45.696	28.788	1.00	20.00
ATOM	1077	CG	GLN A 940	51.695	46.374	27.506	1.00	20.00
ATOM	1078	CD	GLN A 940	52.703	45.592	26.720	1.00	20.00
ATOM	1079	OE1	GLN A 940	52.680	45.571	25.496	1.00	20.00
ATOM	1080	NE2	GLN A 940	53.591	44.934	27.418	1.00	20.00
ATOM	1084	N	LEU A 941	52.523	47.832	30.887	1.00	20.00
ATOM	1085	CA	LEU A 941	52.918	49.212	31.110	1.00	20.00
ATOM	1086	C	LEU A 941	54.285	49.397	31.744	1.00	20.00
ATOM	1087	O	LEU A 941	55.074	50.181	31.231	1.00	20.00
ATOM	1088	CB	LEU A 941	51.855	49.924	31.933	1.00	20.00
ATOM	1089	CG	LEU A 941	50.700	50.500	31.161	1.00	20.00
ATOM	1090	CD1	LEU A 941	50.187	51.653	31.924	1.00	20.00
ATOM	1091	CD2	LEU A 941	51.139	50.904	29.785	1.00	20.00
ATOM	1093	N	LEU A 942	54.571	48.720	32.848	1.00	20.00
ATOM	1094	CA	LEU A 942	55.882	48.863	33.431	1.00	20.00
ATOM	1095	C	LEU A 942	56.822	48.204	32.440	1.00	20.00
ATOM	1096	O	LEU A 942	57.987	48.583	32.283	1.00	20.00
ATOM	1097	CB	LEU A 942	55.955	48.147	34.756	1.00	20.00
ATOM	1098	CG	LEU A 942	54.731	48.399	35.609	1.00	20.00
ATOM	1099	CD1	LEU A 942	54.907	47.676	36.943	1.00	20.00
ATOM	1100	CD2	LEU A 942	54.526	49.936	35.793	1.00	20.00
ATOM	1102	N	HIS A 943	56.309	47.201	31.761	1.00	20.00
ATOM	1103	CA	HIS A 943	57.127	46.548	30.800	1.00	20.00
ATOM	1104	C	HIS A 943	57.754	47.596	29.894	1.00	20.00
ATOM	1105	O	HIS A 943	58.969	47.781	29.936	1.00	20.00
ATOM	1106	CB	HIS A 943	56.302	45.586	29.997	1.00	20.00
ATOM	1107	CG	HIS A 943	56.549	44.159	30.350	1.00	20.00
ATOM	1108	ND1	HIS A 943	56.709	43.732	31.649	1.00	20.00
ATOM	1109	CD2	HIS A 943	56.634	43.054	29.582	1.00	20.00
ATOM	1110	CE1	HIS A 943	56.881	42.427	31.670	1.00	20.00
ATOM	1111	NE2	HIS A 943	56.841	41.994	30.427	1.00	20.00
ATOM	1115	N	PHE A 944	56.929	48.278	29.084	1.00	20.00
ATOM	1116	CA	PHE A 944	57.396	49.327	28.162	1.00	20.00
ATOM	1117	C	PHE A 944	58.366	50.354	28.831	1.00	20.00
ATOM	1118	O	PHE A 944	59.368	50.775	28.249	1.00	20.00

FIG. 4P

ATOM	1119	CB	PHE	A	944	56.205	50.071	27.619	1.00	20.00
ATOM	1120	CG	PHE	A	944	55.484	49.372	26.515	1.00	20.00
ATOM	1121	CD1	PHE	A	944	54.116	49.207	26.572	1.00	20.00
ATOM	1122	CD2	PHE	A	944	56.130	49.020	25.368	1.00	20.00
ATOM	1123	CE1	PHE	A	944	53.432	48.727	25.515	1.00	20.00
ATOM	1124	CE2	PHE	A	944	55.433	48.534	24.300	1.00	20.00
ATOM	1125	CZ	PHE	A	944	54.096	48.393	24.375	1.00	20.00
ATOM	1127	N	ALA	A	945	58.055	50.749	30.057	1.00	20.00
ATOM	1128	CA	ALA	A	945	58.919	51.639	30.792	1.00	20.00
ATOM	1129	C	ALA	A	945	60.323	51.010	31.013	1.00	20.00
ATOM	1130	O	ALA	A	945	61.349	51.690	30.906	1.00	20.00
ATOM	1131	CB	ALA	A	945	58.292	51.974	32.101	1.00	20.00
ATOM	1133	N	ALA	A	946	60.373	49.710	31.297	1.00	20.00
ATOM	1134	CA	ALA	A	946	61.650	49.043	31.547	1.00	20.00
ATOM	1135	C	ALA	A	946	62.466	48.605	30.330	1.00	20.00
ATOM	1136	O	ALA	A	946	63.646	48.331	30.434	1.00	20.00
ATOM	1137	CB	ALA	A	946	61.418	47.872	32.429	1.00	20.00
ATOM	1139	N	ASP	A	947	61.823	48.486	29.188	1.00	20.00
ATOM	1140	CA	ASP	A	947	62.532	48.106	27.998	1.00	20.00
ATOM	1141	C	ASP	A	947	63.351	49.335	27.765	1.00	20.00
ATOM	1142	O	ASP	A	947	64.564	49.273	27.560	1.00	20.00
ATOM	1143	CB	ASP	A	947	61.560	47.930	26.849	1.00	20.00
ATOM	1144	CG	ASP	A	947	61.242	46.473	26.549	1.00	20.00
ATOM	1145	OD1	ASP	A	947	61.770	45.561	27.247	1.00	20.00
ATOM	1146	OD2	ASP	A	947	60.447	46.255	25.595	1.00	20.00
ATOM	1148	N	VAL	A	948	62.640	50.465	27.811	1.00	20.00
ATOM	1149	CA	VAL	A	948	63.203	51.808	27.624	1.00	20.00
ATOM	1150	C	VAL	A	948	64.337	52.099	28.598	1.00	20.00
ATOM	1151	O	VAL	A	948	65.360	52.539	28.177	1.00	20.00
ATOM	1152	CB	VAL	A	948	62.108	52.917	27.776	1.00	20.00
ATOM	1153	CG1	VAL	A	948	62.712	54.286	27.666	1.00	20.00
ATOM	1154	CG2	VAL	A	948	61.121	52.784	26.722	1.00	20.00
ATOM	1156	N	ALA	A	949	64.166	51.850	29.886	1.00	20.00
ATOM	1157	CA	ALA	A	949	65.243	52.135	30.812	1.00	20.00
ATOM	1158	C	ALA	A	949	66.449	51.321	30.460	1.00	20.00
ATOM	1159	O	ALA	A	949	67.578	51.738	30.669	1.00	20.00
ATOM	1160	CB	ALA	A	949	64.850	51.822	32.209	1.00	20.00
ATOM	1162	N	ARG	A	950	66.212	50.134	29.928	1.00	20.00
ATOM	1163	CA	ARG	A	950	67.293	49.254	29.578	1.00	20.00
ATOM	1164	C	ARG	A	950	68.005	49.853	28.406	1.00	20.00
ATOM	1165	O	ARG	A	950	69.110	50.330	28.534	1.00	20.00
ATOM	1166	CB	ARG	A	950	66.762	47.872	29.240	1.00	20.00
ATOM	1167	CG	ARG	A	950	67.029	46.827	30.351	1.00	20.00
ATOM	1168	CD	ARG	A	950	67.033	45.384	29.809	1.00	20.00
ATOM	1169	NE	ARG	A	950	65.891	45.157	28.900	1.00	20.00
ATOM	1170	CZ	ARG	A	950	64.646	44.807	29.260	1.00	20.00
ATOM	1171	NH1	ARG	A	950	64.301	44.610	30.522	1.00	20.00
ATOM	1172	NH2	ARG	A	950	63.726	44.693	28.323	1.00	20.00
ATOM	1179	N	GLY	A	951	67.390	49.844	27.248	1.00	20.00
ATOM	1180	CA	GLY	A	951	68.105	50.427	26.146	1.00	20.00
ATOM	1181	C	GLY	A	951	68.769	51.722	26.564	1.00	20.00
ATOM	1182	O	GLY	A	951	69.885	52.024	26.163	1.00	20.00
ATOM	1184	N	MET	A	952	68.080	52.500	27.386	1.00	20.00
ATOM	1185	CA	MET	A	952	68.605	53.787	27.807	1.00	20.00
ATOM	1186	C	MET	A	952	69.952	53.633	28.437	1.00	20.00
ATOM	1187	O	MET	A	952	70.949	53.969	27.845	1.00	20.00
ATOM	1188	CB	MET	A	952	67.659	54.492	28.797	1.00	20.00

FIG. 4Q

ATOM	1189	CG	MET	A	952	67.289	55.894	28.400	1.00	20.00
ATOM	1190	SD	MET	A	952	67.360	56.078	26.632	1.00	20.00
ATOM	1191	CE	MET	A	952	68.656	57.374	26.554	1.00	20.00
ATOM	1193	N	ASP	A	953	69.903	53.096	29.648	1.00	20.00
ATOM	1194	CA	ASP	A	953	70.999	52.819	30.539	1.00	20.00
ATOM	1195	C	ASP	A	953	72.126	52.077	29.948	1.00	20.00
ATOM	1196	O	ASP	A	953	73.077	51.814	30.608	1.00	20.00
ATOM	1197	CB	ASP	A	953	70.496	52.036	31.733	1.00	20.00
ATOM	1198	CG	ASP	A	953	71.538	51.117	32.295	1.00	20.00
ATOM	1199	OD1	ASP	A	953	72.241	51.480	33.245	1.00	20.00
ATOM	1200	OD2	ASP	A	953	71.672	50.004	31.785	1.00	20.00
ATOM	1202	N	TYR	A	954	72.025	51.743	28.692	1.00	20.00
ATOM	1203	CA	TYR	A	954	73.060	51.020	28.034	1.00	20.00
ATOM	1204	C	TYR	A	954	73.930	52.011	27.324	1.00	20.00
ATOM	1205	O	TYR	A	954	75.135	51.833	27.254	1.00	20.00
ATOM	1206	CB	TYR	A	954	72.416	50.047	27.070	1.00	20.00
ATOM	1207	CG	TYR	A	954	73.330	49.432	26.068	1.00	20.00
ATOM	1208	CD1	TYR	A	954	74.294	48.485	26.442	1.00	20.00
ATOM	1209	CD2	TYR	A	954	73.181	49.719	24.734	1.00	20.00
ATOM	1210	CE1	TYR	A	954	75.071	47.839	25.483	1.00	20.00
ATOM	1211	CE2	TYR	A	954	73.947	49.082	23.779	1.00	20.00
ATOM	1212	CZ	TYR	A	954	74.883	48.136	24.153	1.00	20.00
ATOM	1213	OH	TYR	A	954	75.525	47.442	23.152	1.00	20.00
ATOM	1216	N	LEU	A	955	73.286	53.052	26.786	1.00	20.00
ATOM	1217	CA	LEU	A	955	73.908	54.184	26.069	1.00	20.00
ATOM	1218	C	LEU	A	955	74.356	55.110	27.176	1.00	20.00
ATOM	1219	O	LEU	A	955	75.441	55.609	27.207	1.00	20.00
ATOM	1220	CB	LEU	A	955	72.863	54.943	25.265	1.00	20.00
ATOM	1221	CG	LEU	A	955	72.005	54.277	24.181	1.00	20.00
ATOM	1222	CD1	LEU	A	955	70.489	54.637	24.288	1.00	20.00
ATOM	1223	CD2	LEU	A	955	72.573	54.751	22.838	1.00	20.00
ATOM	1225	N	SER	A	956	73.465	55.311	28.113	1.00	20.00
ATOM	1226	CA	SER	A	956	73.699	56.176	29.209	1.00	20.00
ATOM	1227	C	SER	A	956	74.985	55.783	29.829	1.00	20.00
ATOM	1228	O	SER	A	956	75.557	56.555	30.600	1.00	20.00
ATOM	1229	CB	SER	A	956	72.534	56.068	30.172	1.00	20.00
ATOM	1230	OG	SER	A	956	72.960	56.102	31.513	1.00	20.00
ATOM	1233	N	GLN	A	957	75.468	54.594	29.495	1.00	20.00
ATOM	1234	CA	GLN	A	957	76.755	54.097	30.040	1.00	20.00
ATOM	1235	C	GLN	A	957	77.824	54.054	28.959	1.00	20.00
ATOM	1236	O	GLN	A	957	78.985	54.213	29.208	1.00	20.00
ATOM	1237	CB	GLN	A	957	76.591	52.703	30.617	1.00	20.00
ATOM	1238	CG	GLN	A	957	75.563	52.626	31.692	1.00	20.00
ATOM	1239	CD	GLN	A	957	76.088	51.882	32.875	1.00	20.00
ATOM	1240	OE1	GLN	A	957	77.083	52.314	33.492	1.00	20.00
ATOM	1241	NE2	GLN	A	957	75.447	50.747	33.215	1.00	20.00
ATOM	1245	N	LYS	A	958	77.396	53.827	27.747	1.00	20.00
ATOM	1246	CA	LYS	A	958	78.273	53.813	26.622	1.00	20.00
ATOM	1247	C	LYS	A	958	78.801	55.275	26.542	1.00	20.00
ATOM	1248	O	LYS	A	958	79.643	55.627	25.704	1.00	20.00
ATOM	1249	CB	LYS	A	958	77.427	53.440	25.379	1.00	20.00
ATOM	1250	CG	LYS	A	958	78.110	52.552	24.355	1.00	20.00
ATOM	1251	CD	LYS	A	958	78.715	51.303	25.011	1.00	20.00
ATOM	1252	CE	LYS	A	958	77.845	50.099	24.743	1.00	20.00
ATOM	1253	NZ	LYS	A	958	77.570	50.041	23.271	1.00	20.00
ATOM	1258	N	GLN	A	959	78.268	56.108	27.438	1.00	20.00
ATOM	1259	CA	GLN	A	959	78.526	57.551	27.543	1.00	20.00

FIG. 4R

ATOM	1260	C	GLN	A	959	77.366	58.361	26.838	1.00	20.00
ATOM	1261	O	GLN	A	959	76.848	59.327	27.401	1.00	20.00
ATOM	1262	CB	GLN	A	959	79.901	57.893	26.973	1.00	20.00
ATOM	1263	CG	GLN	A	959	80.490	59.183	27.492	1.00	20.00
ATOM	1264	CD	GLN	A	959	80.934	59.114	28.944	1.00	20.00
ATOM	1265	OE1	GLN	A	959	81.840	58.313	29.295	1.00	20.00
ATOM	1266	NE2	GLN	A	959	80.332	59.979	29.811	1.00	20.00
ATOM	1270	N	PHE	A	960	76.937	57.940	25.649	1.00	20.00
ATOM	1271	CA	PHE	A	960	75.828	58.582	24.898	1.00	20.00
ATOM	1272	C	PHE	A	960	74.667	59.365	25.618	1.00	20.00
ATOM	1273	O	PHE	A	960	74.110	58.916	26.628	1.00	20.00
ATOM	1274	CB	PHE	A	960	75.189	57.528	23.985	1.00	20.00
ATOM	1275	CG	PHE	A	960	76.070	57.067	22.851	1.00	20.00
ATOM	1276	CD1	PHE	A	960	76.570	55.766	22.818	1.00	20.00
ATOM	1277	CD2	PHE	A	960	76.367	57.901	21.792	1.00	20.00
ATOM	1278	CE1	PHE	A	960	77.349	55.308	21.743	1.00	20.00
ATOM	1279	CE2	PHE	A	960	77.148	57.442	20.720	1.00	20.00
ATOM	1280	CZ	PHE	A	960	77.636	56.142	20.704	1.00	20.00
ATOM	1282	N	ILE	A	961	74.308	60.532	25.068	1.00	20.00
ATOM	1283	CA	ILE	A	961	73.212	61.377	25.623	1.00	20.00
ATOM	1284	C	ILE	A	961	72.076	61.460	24.611	1.00	20.00
ATOM	1285	O	ILE	A	961	72.341	61.698	23.434	1.00	20.00
ATOM	1286	CB	ILE	A	961	73.631	62.832	25.918	1.00	20.00
ATOM	1287	CG1	ILE	A	961	74.862	62.886	26.840	1.00	20.00
ATOM	1288	CG2	ILE	A	961	72.489	63.547	26.600	1.00	20.00
ATOM	1289	CD1	ILE	A	961	75.935	63.855	26.373	1.00	20.00
ATOM	1291	N	HIS	A	962	70.821	61.314	25.049	1.00	20.00
ATOM	1292	CA	HIS	A	962	69.704	61.307	24.088	1.00	20.00
ATOM	1293	C	HIS	A	962	69.158	62.604	23.535	1.00	20.00
ATOM	1294	O	HIS	A	962	69.296	62.872	22.344	1.00	20.00
ATOM	1295	CB	HIS	A	962	68.515	60.516	24.641	1.00	20.00
ATOM	1296	CG	HIS	A	962	67.658	59.896	23.580	1.00	20.00
ATOM	1297	ND1	HIS	A	962	67.259	58.586	23.621	1.00	20.00
ATOM	1298	CD2	HIS	A	962	67.192	60.388	22.416	1.00	20.00
ATOM	1299	CE1	HIS	A	962	66.589	58.290	22.528	1.00	20.00
ATOM	1300	NE2	HIS	A	962	66.538	59.369	21.780	1.00	20.00
ATOM	1304	N	ARG	A	963	68.502	63.363	24.413	1.00	20.00
ATOM	1305	CA	ARG	A	963	67.848	64.665	24.122	1.00	20.00
ATOM	1306	C	ARG	A	963	66.653	64.636	23.125	1.00	20.00
ATOM	1307	O	ARG	A	963	66.561	65.380	22.147	1.00	20.00
ATOM	1308	CB	ARG	A	963	68.909	65.724	23.726	1.00	20.00
ATOM	1309	CG	ARG	A	963	69.366	65.645	22.334	1.00	20.00
ATOM	1310	CD	ARG	A	963	70.710	66.180	22.216	1.00	20.00
ATOM	1311	NE	ARG	A	963	71.391	65.521	21.127	1.00	20.00
ATOM	1312	CZ	ARG	A	963	71.002	65.603	19.873	1.00	20.00
ATOM	1313	NH1	ARG	A	963	69.946	66.323	19.584	1.00	20.00
ATOM	1314	NH2	ARG	A	963	71.648	64.941	18.925	1.00	20.00
ATOM	1321	N	ASN	A	964	65.705	63.767	23.408	1.00	20.00
ATOM	1322	CA	ASN	A	964	64.536	63.623	22.545	1.00	20.00
ATOM	1323	C	ASN	A	964	63.904	62.262	22.803	1.00	20.00
ATOM	1324	O	ASN	A	964	63.497	61.558	21.890	1.00	20.00
ATOM	1325	CB	ASN	A	964	64.890	63.763	21.054	1.00	20.00
ATOM	1326	CG	ASN	A	964	63.647	63.940	20.206	1.00	20.00
ATOM	1327	OD1	ASN	A	964	62.565	64.079	20.780	1.00	20.00
ATOM	1328	ND2	ASN	A	964	63.769	63.939	18.866	1.00	20.00
ATOM	1332	N	LEU	A	965	63.861	61.914	24.081	1.00	20.00
ATOM	1333	CA	LEU	A	965	63.291	60.665	24.546	1.00	20.00

FIG. 4S

ATOM	1334	C	LEU A 965	61.884	61.116	24.926	1.00	20.00
ATOM	1335	O	LEU A 965	61.701	62.119	25.629	1.00	20.00
ATOM	1336	CB	LEU A 965	64.079	60.172	25.769	1.00	20.00
ATOM	1337	CG	LEU A 965	64.292	58.716	26.189	1.00	20.00
ATOM	1338	CD1	LEU A 965	64.689	57.802	25.040	1.00	20.00
ATOM	1339	CD2	LEU A 965	65.320	58.728	27.276	1.00	20.00
ATOM	1341	N	ALA A 966	60.905	60.381	24.412	1.00	20.00
ATOM	1342	CA	ALA A 966	59.511	60.666	24.605	1.00	20.00
ATOM	1343	C	ALA A 966	58.812	59.674	23.677	1.00	20.00
ATOM	1344	O	ALA A 966	59.379	59.250	22.667	1.00	20.00
ATOM	1345	CB	ALA A 966	59.244	62.056	24.189	1.00	20.00
ATOM	1347	N	ALA A 967	57.581	59.320	24.014	1.00	20.00
ATOM	1348	CA	ALA A 967	56.826	58.358	23.242	1.00	20.00
ATOM	1349	C	ALA A 967	56.842	58.489	21.740	1.00	20.00
ATOM	1350	O	ALA A 967	57.050	57.521	21.044	1.00	20.00
ATOM	1351	CB	ALA A 967	55.375	58.306	23.721	1.00	20.00
ATOM	1353	N	ARG A 968	56.606	59.671	21.205	1.00	20.00
ATOM	1354	CA	ARG A 968	56.580	59.697	19.759	1.00	20.00
ATOM	1355	C	ARG A 968	57.802	59.015	19.160	1.00	20.00
ATOM	1356	O	ARG A 968	57.751	58.532	18.041	1.00	20.00
ATOM	1357	CB	ARG A 968	56.455	61.123	19.226	1.00	20.00
ATOM	1358	CG	ARG A 968	57.264	62.162	19.987	1.00	20.00
ATOM	1359	CD	ARG A 968	57.684	63.354	19.087	1.00	20.00
ATOM	1360	NE	ARG A 968	58.467	64.376	19.784	1.00	20.00
ATOM	1361	CZ	ARG A 968	58.098	64.982	20.904	1.00	20.00
ATOM	1362	NH1	ARG A 968	56.937	64.698	21.492	1.00	20.00
ATOM	1363	NH2	ARG A 968	58.929	65.828	21.473	1.00	20.00
ATOM	1370	N	ASN A 969	58.881	58.913	19.931	1.00	20.00
ATOM	1371	CA	ASN A 969	60.122	58.388	19.383	1.00	20.00
ATOM	1372	C	ASN A 969	60.608	57.008	19.754	1.00	20.00
ATOM	1373	O	ASN A 969	61.716	56.647	19.413	1.00	20.00
ATOM	1374	CB	ASN A 969	61.232	59.407	19.630	1.00	20.00
ATOM	1375	CG	ASN A 969	60.873	60.787	19.118	1.00	20.00
ATOM	1376	OD1	ASN A 969	60.733	61.724	19.892	1.00	20.00
ATOM	1377	ND2	ASN A 969	60.702	60.910	17.802	1.00	20.00
ATOM	1381	N	ILE A 970	59.775	56.249	20.443	1.00	20.00
ATOM	1382	CA	ILE A 970	60.073	54.912	20.851	1.00	20.00
ATOM	1383	C	ILE A 970	59.153	54.057	20.034	1.00	20.00
ATOM	1384	O	ILE A 970	58.006	54.384	19.930	1.00	20.00
ATOM	1385	CB	ILE A 970	59.717	54.770	22.294	1.00	20.00
ATOM	1386	CG1	ILE A 970	60.699	55.565	23.110	1.00	20.00
ATOM	1387	CG2	ILE A 970	59.730	53.328	22.724	1.00	20.00
ATOM	1388	CD1	ILE A 970	60.800	55.095	24.515	1.00	20.00
ATOM	1390	N	LEU A 971	59.626	52.971	19.435	1.00	20.00
ATOM	1391	CA	LEU A 971	58.733	52.086	18.656	1.00	20.00
ATOM	1392	C	LEU A 971	58.290	50.891	19.444	1.00	20.00
ATOM	1393	O	LEU A 971	58.776	50.653	20.523	1.00	20.00
ATOM	1394	CB	LEU A 971	59.422	51.582	17.418	1.00	20.00
ATOM	1395	CG	LEU A 971	59.930	52.837	16.785	1.00	20.00
ATOM	1396	CD1	LEU A 971	61.161	52.652	16.019	1.00	20.00
ATOM	1397	CD2	LEU A 971	58.844	53.290	15.909	1.00	20.00
ATOM	1399	N	VAL A 972	57.305	50.171	18.929	1.00	20.00
ATOM	1400	CA	VAL A 972	56.894	48.941	19.594	1.00	20.00
ATOM	1401	C	VAL A 972	57.044	47.883	18.541	1.00	20.00
ATOM	1402	O	VAL A 972	56.221	47.793	17.661	1.00	20.00
ATOM	1403	CB	VAL A 972	55.492	48.932	20.043	1.00	20.00
ATOM	1404	CG1	VAL A 972	55.224	47.588	20.632	1.00	20.00

FIG. 4T

ATOM	1405	CG2	VAL	A	972	55.264	50.012	21.107	1.00	20.00
ATOM	1407	N	GLY	A	973	58.127	47.106	18.614	1.00	20.00
ATOM	1408	CA	GLY	A	973	58.375	46.109	17.614	1.00	20.00
ATOM	1409	C	GLY	A	973	58.065	44.685	17.980	1.00	20.00
ATOM	1410	O	GLY	A	973	57.370	44.393	18.927	1.00	20.00
ATOM	1412	N	GLU	A	974	58.612	43.793	17.178	1.00	20.00
ATOM	1413	CA	GLU	A	974	58.445	42.383	17.357	1.00	20.00
ATOM	1414	C	GLU	A	974	58.379	41.981	18.795	1.00	20.00
ATOM	1415	O	GLU	A	974	59.246	42.274	19.572	1.00	20.00
ATOM	1416	CB	GLU	A	974	59.568	41.648	16.671	1.00	20.00
ATOM	1417	CG	GLU	A	974	59.187	41.010	15.343	1.00	20.00
ATOM	1418	CD	GLU	A	974	57.698	41.173	14.936	1.00	20.00
ATOM	1419	OE1	GLU	A	974	56.763	40.870	15.733	1.00	20.00
ATOM	1420	OE2	GLU	A	974	57.467	41.592	13.780	1.00	20.00
ATOM	1422	N	ASN	A	975	57.305	41.316	19.147	1.00	20.00
ATOM	1423	CA	ASN	A	975	57.119	40.830	20.483	1.00	20.00
ATOM	1424	C	ASN	A	975	56.741	41.832	21.554	1.00	20.00
ATOM	1425	O	ASN	A	975	56.811	41.544	22.758	1.00	20.00
ATOM	1426	CB	ASN	A	975	58.333	40.006	20.864	1.00	20.00
ATOM	1427	CG	ASN	A	975	58.189	38.519	20.428	1.00	20.00
ATOM	1428	OD1	ASN	A	975	58.243	37.639	21.263	1.00	20.00
ATOM	1429	ND2	ASN	A	975	57.988	38.266	19.136	1.00	20.00
ATOM	1433	N	TYR	A	976	56.299	43.003	21.103	1.00	20.00
ATOM	1434	CA	TYR	A	976	55.839	44.047	21.988	1.00	20.00
ATOM	1435	C	TYR	A	976	56.946	44.589	22.839	1.00	20.00
ATOM	1436	O	TYR	A	976	56.797	44.863	24.016	1.00	20.00
ATOM	1437	CB	TYR	A	976	54.684	43.498	22.830	1.00	20.00
ATOM	1438	CG	TYR	A	976	53.466	43.191	21.993	1.00	20.00
ATOM	1439	CD1	TYR	A	976	52.878	41.927	22.017	1.00	20.00
ATOM	1440	CD2	TYR	A	976	52.939	44.157	21.112	1.00	20.00
ATOM	1441	CE1	TYR	A	976	51.801	41.624	21.182	1.00	20.00
ATOM	1442	CE2	TYR	A	976	51.874	43.870	20.279	1.00	20.00
ATOM	1443	CZ	TYR	A	976	51.306	42.604	20.307	1.00	20.00
ATOM	1444	OH	TYR	A	976	50.273	42.291	19.427	1.00	20.00
ATOM	1447	N	VAL	A	977	58.070	44.787	22.191	1.00	20.00
ATOM	1448	CA	VAL	A	977	59.260	45.295	22.845	1.00	20.00
ATOM	1449	C	VAL	A	977	59.536	46.766	22.497	1.00	20.00
ATOM	1450	O	VAL	A	977	59.446	47.195	21.355	1.00	20.00
ATOM	1451	CB	VAL	A	977	60.514	44.377	22.485	1.00	20.00
ATOM	1452	CG1	VAL	A	977	61.768	44.854	23.182	1.00	20.00
ATOM	1453	CG2	VAL	A	977	60.230	42.943	22.890	1.00	20.00
ATOM	1455	N	ALA	A	978	59.839	47.529	23.525	1.00	20.00
ATOM	1456	CA	ALA	A	978	60.174	48.898	23.328	1.00	20.00
ATOM	1457	C	ALA	A	978	61.434	48.921	22.476	1.00	20.00
ATOM	1458	O	ALA	A	978	62.242	48.026	22.527	1.00	20.00
ATOM	1459	CB	ALA	A	978	60.423	49.546	24.643	1.00	20.00
ATOM	1461	N	LYS	A	979	61.597	49.926	21.653	1.00	20.00
ATOM	1462	CA	LYS	A	979	62.791	50.005	20.864	1.00	20.00
ATOM	1463	C	LYS	A	979	63.098	51.476	20.826	1.00	20.00
ATOM	1464	O	LYS	A	979	62.263	52.262	20.387	1.00	20.00
ATOM	1465	CB	LYS	A	979	62.551	49.492	19.448	1.00	20.00
ATOM	1466	CG	LYS	A	979	62.076	48.043	19.369	1.00	20.00
ATOM	1467	CD	LYS	A	979	63.115	47.009	19.864	1.00	20.00
ATOM	1468	CE	LYS	A	979	63.866	46.343	18.708	1.00	20.00
ATOM	1469	NZ	LYS	A	979	63.212	45.122	18.253	1.00	20.00
ATOM	1474	N	ILE	A	980	64.274	51.873	21.302	1.00	20.00
ATOM	1475	CA	ILE	A	980	64.615	53.287	21.240	1.00	20.00

FIG. 4U

ATOM	1476	C	ILE	A	980	65.131	53.691	19.858	1.00	20.00
ATOM	1477	O	ILE	A	980	65.938	53.004	19.233	1.00	20.00
ATOM	1478	CB	ILE	A	980	65.671	53.665	22.263	1.00	20.00
ATOM	1479	CG1	ILE	A	980	65.205	53.311	23.667	1.00	20.00
ATOM	1480	CG2	ILE	A	980	65.943	55.135	22.173	1.00	20.00
ATOM	1481	CD1	ILE	A	980	66.262	53.521	24.730	1.00	20.00
ATOM	1483	N	ALA	A	981	64.629	54.815	19.383	1.00	20.00
ATOM	1484	CA	ALA	A	981	65.038	55.342	18.097	1.00	20.00
ATOM	1485	C	ALA	A	981	65.244	56.854	18.141	1.00	20.00
ATOM	1486	O	ALA	A	981	65.039	57.530	19.172	1.00	20.00
ATOM	1487	CB	ALA	A	981	64.024	55.024	17.060	1.00	20.00
ATOM	1489	N	ASP	A	982	65.610	57.362	16.973	1.00	20.00
ATOM	1490	CA	ASP	A	982	65.888	58.763	16.721	1.00	20.00
ATOM	1491	C	ASP	A	982	66.653	59.517	17.801	1.00	20.00
ATOM	1492	O	ASP	A	982	66.041	60.135	18.684	1.00	20.00
ATOM	1493	CB	ASP	A	982	64.620	59.527	16.416	1.00	20.00
ATOM	1494	CG	ASP	A	982	64.911	60.946	16.122	1.00	20.00
ATOM	1495	OD1	ASP	A	982	65.455	61.240	15.031	1.00	20.00
ATOM	1496	OD2	ASP	A	982	64.626	61.766	16.998	1.00	20.00
ATOM	1498	N	PHE	A	983	67.988	59.525	17.706	1.00	20.00
ATOM	1499	CA	PHE	A	983	68.770	60.223	18.733	1.00	20.00
ATOM	1500	C	PHE	A	983	70.123	60.755	18.312	1.00	20.00
ATOM	1501	O	PHE	A	983	70.565	60.712	17.155	1.00	20.00
ATOM	1502	CB	PHE	A	983	69.001	59.327	19.948	1.00	20.00
ATOM	1503	CG	PHE	A	983	69.411	57.928	19.589	1.00	20.00
ATOM	1504	CD1	PHE	A	983	68.856	57.280	18.452	1.00	20.00
ATOM	1505	CD2	PHE	A	983	70.310	57.244	20.375	1.00	20.00
ATOM	1506	CE1	PHE	A	983	69.181	55.987	18.106	1.00	20.00
ATOM	1507	CE2	PHE	A	983	70.648	55.939	20.044	1.00	20.00
ATOM	1508	CZ	PHE	A	983	70.075	55.308	18.895	1.00	20.00
ATOM	1510	N	GLY	A	984	70.797	61.274	19.305	1.00	20.00
ATOM	1511	CA	GLY	A	984	72.082	61.799	19.010	1.00	20.00
ATOM	1512	C	GLY	A	984	73.058	60.661	18.913	1.00	20.00
ATOM	1513	O	GLY	A	984	72.980	59.633	19.633	1.00	20.00
ATOM	1515	N	LEU	A	985	73.978	60.846	17.977	1.00	20.00
ATOM	1516	CA	LEU	A	985	75.055	59.913	17.812	1.00	20.00
ATOM	1517	C	LEU	A	985	76.044	60.741	18.669	1.00	20.00
ATOM	1518	O	LEU	A	985	77.236	60.872	18.323	1.00	20.00
ATOM	1519	CB	LEU	A	985	75.483	59.871	16.342	1.00	20.00
ATOM	1520	CG	LEU	A	985	75.093	58.770	15.337	1.00	20.00
ATOM	1521	CD1	LEU	A	985	75.645	57.463	15.830	1.00	20.00
ATOM	1522	CD2	LEU	A	985	73.579	58.659	15.129	1.00	20.00
ATOM	1524	N	SER	A	986	75.561	61.306	19.786	1.00	20.00
ATOM	1525	CA	SER	A	986	76.443	62.118	20.611	1.00	20.00
ATOM	1526	C	SER	A	986	76.926	61.629	21.970	1.00	20.00
ATOM	1527	O	SER	A	986	76.169	61.709	22.937	1.00	20.00
ATOM	1528	CB	SER	A	986	75.850	63.504	20.815	1.00	20.00
ATOM	1529	OG	SER	A	986	76.764	64.504	20.379	1.00	20.00
ATOM	1532	N	ARG	A	987	78.189	61.152	22.037	1.00	20.00
ATOM	1533	CA	ARG	A	987	78.763	60.709	23.306	1.00	20.00
ATOM	1534	C	ARG	A	987	79.511	61.893	23.794	1.00	20.00
ATOM	1535	O	ARG	A	987	80.191	62.578	23.059	1.00	20.00
ATOM	1536	CB	ARG	A	987	79.752	59.525	23.214	1.00	20.00
ATOM	1537	CG	ARG	A	987	79.583	58.534	22.078	1.00	20.00
ATOM	1538	CD	ARG	A	987	80.953	58.120	21.459	1.00	20.00
ATOM	1539	NE	ARG	A	987	81.908	57.509	22.396	1.00	20.00
ATOM	1540	CZ	ARG	A	987	82.932	56.731	22.021	1.00	20.00

FIG. 4V

ATOM	1541	NH1	ARG	A	987	83.127	56.473	20.738	1.00	20.00
ATOM	1542	NH2	ARG	A	987	83.761	56.206	22.936	1.00	20.00
ATOM	1549	N	GLY	A	988	79.387	62.122	25.068	1.00	20.00
ATOM	1550	CA	GLY	A	988	80.028	63.260	25.633	1.00	20.00
ATOM	1551	C	GLY	A	988	79.480	63.223	27.024	1.00	20.00
ATOM	1552	O	GLY	A	988	79.050	62.151	27.453	1.00	20.00
ATOM	1554	N	GLN	A	989	79.521	64.369	27.704	1.00	20.00
ATOM	1555	CA	GLN	A	989	79.020	64.579	29.053	1.00	20.00
ATOM	1556	C	GLN	A	989	78.115	65.864	29.062	1.00	20.00
ATOM	1557	O	GLN	A	989	77.565	66.257	30.075	1.00	20.00
ATOM	1558	CB	GLN	A	989	80.219	64.739	29.974	1.00	20.00
ATOM	1559	CG	GLN	A	989	79.924	65.292	31.348	1.00	20.00
ATOM	1560	CD	GLN	A	989	81.068	66.095	31.985	1.00	20.00
ATOM	1561	OE1	GLN	A	989	81.783	66.897	31.332	1.00	20.00
ATOM	1562	NE2	GLN	A	989	81.233	65.891	33.273	1.00	20.00
ATOM	1566	N	GLU	A	990	77.933	66.496	27.908	1.00	20.00
ATOM	1567	CA	GLU	A	990	77.185	67.704	27.889	1.00	20.00
ATOM	1568	C	GLU	A	990	76.348	68.030	26.675	1.00	20.00
ATOM	1569	O	GLU	A	990	75.199	68.420	26.836	1.00	20.00
ATOM	1570	CB	GLU	A	990	78.134	68.853	28.117	1.00	20.00
ATOM	1571	CG	GLU	A	990	78.194	69.367	29.499	1.00	20.00
ATOM	1572	CD	GLU	A	990	79.467	68.991	30.151	1.00	20.00
ATOM	1573	OE1	GLU	A	990	80.437	68.623	29.443	1.00	20.00
ATOM	1574	OE2	GLU	A	990	79.486	69.061	31.387	1.00	20.00
ATOM	1576	N	VAL	A	991	76.878	67.895	25.469	1.00	20.00
ATOM	1577	CA	VAL	A	991	76.098	68.270	24.274	1.00	20.00
ATOM	1578	C	VAL	A	991	75.373	69.616	24.400	1.00	20.00
ATOM	1579	O	VAL	A	991	74.538	69.823	25.274	1.00	20.00
ATOM	1580	CB	VAL	A	991	74.965	67.324	23.910	1.00	20.00
ATOM	1581	CG1	VAL	A	991	74.620	67.527	22.479	1.00	20.00
ATOM	1582	CG2	VAL	A	991	75.323	65.922	24.159	1.00	20.00
ATOM	1584	N	TYR	A	992	75.674	70.528	23.504	1.00	20.00
ATOM	1585	CA	TYR	A	992	74.997	71.780	23.514	1.00	20.00
ATOM	1586	C	TYR	A	992	74.389	71.784	22.118	1.00	20.00
ATOM	1587	O	TYR	A	992	75.036	71.437	21.138	1.00	20.00
ATOM	1588	CB	TYR	A	992	76.003	72.945	23.687	1.00	20.00
ATOM	1589	CG	TYR	A	992	75.520	74.227	23.027	1.00	20.00
ATOM	1590	CD1	TYR	A	992	74.579	75.023	23.654	1.00	20.00
ATOM	1591	CD2	TYR	A	992	75.804	74.487	21.702	1.00	20.00
ATOM	1592	CE1	TYR	A	992	73.939	75.989	22.987	1.00	20.00
ATOM	1593	CE2	TYR	A	992	75.160	75.453	21.044	1.00	20.00
ATOM	1594	CZ	TYR	A	992	74.218	76.200	21.690	1.00	20.00
ATOM	1595	OH	TYR	A	992	73.552	77.196	21.023	1.00	20.00
ATOM	1598	N	VAL	A	993	73.131	72.161	22.020	1.00	20.00
ATOM	1599	CA	VAL	A	993	72.482	72.226	20.712	1.00	20.00
ATOM	1600	C	VAL	A	993	71.311	73.168	21.008	1.00	20.00
ATOM	1601	O	VAL	A	993	70.748	73.116	22.101	1.00	20.00
ATOM	1602	CB	VAL	A	993	72.102	70.746	20.159	1.00	20.00
ATOM	1603	CG1	VAL	A	993	71.570	69.843	21.226	1.00	20.00
ATOM	1604	CG2	VAL	A	993	71.121	70.843	19.076	1.00	20.00
ATOM	1606	N	LYS	A	994	70.990	74.076	20.082	1.00	20.00
ATOM	1607	CA	LYS	A	994	69.917	75.099	20.335	1.00	20.00
ATOM	1608	C	LYS	A	994	69.171	75.616	19.093	1.00	20.00
ATOM	1609	O	LYS	A	994	69.784	76.097	18.105	1.00	20.00
ATOM	1610	CB	LYS	A	994	70.508	76.336	21.083	1.00	20.00
ATOM	1611	CG	LYS	A	994	69.513	77.422	21.498	1.00	20.00
ATOM	1612	CD	LYS	A	994	69.827	78.812	20.847	1.00	20.00

FIG. 4W

ATOM	1613	CE	LYS	A	994	69.627	80.017	21.856	1.00	20.00
ATOM	1614	NZ	LYS	A	994	70.649	81.165	21.795	1.00	20.00
ATOM	1619	N	LYS	A	995	67.841	75.573	19.202	1.00	20.00
ATOM	1620	CA	LYS	A	995	66.914	75.962	18.132	1.00	20.00
ATOM	1621	C	LYS	A	995	65.884	74.827	18.184	1.00	20.00
ATOM	1622	O	LYS	A	995	65.303	74.470	17.139	1.00	20.00
ATOM	1623	CB	LYS	A	995	67.633	75.996	16.736	1.00	20.00
ATOM	1624	OXT	LYS	A	995	65.718	74.295	19.306	1.00	20.00
ATOM	1626	N	PRO	A	001	59.536	69.751	22.343	1.00	20.00
ATOM	1627	CA	PRO	A	001	60.339	69.285	23.473	1.00	20.00
ATOM	1628	C	PRO	A	001	60.137	70.032	24.772	1.00	20.00
ATOM	1629	O	PRO	A	001	60.361	69.470	25.821	1.00	20.00
ATOM	1630	CB	PRO	A	001	61.803	69.328	23.049	1.00	20.00
ATOM	1631	CG	PRO	A	001	61.735	69.311	21.525	1.00	20.00
ATOM	1632	CD	PRO	A	001	60.238	69.446	21.080	1.00	20.00
ATOM	1635	N	VAL	A	002	59.712	71.287	24.728	1.00	20.00
ATOM	1636	CA	VAL	A	002	59.503	72.082	25.958	1.00	20.00
ATOM	1637	C	VAL	A	002	58.748	71.338	27.019	1.00	20.00
ATOM	1638	O	VAL	A	002	58.868	71.595	28.206	1.00	20.00
ATOM	1639	CB	VAL	A	002	58.690	73.333	25.706	1.00	20.00
ATOM	1640	CG1	VAL	A	002	58.862	74.285	26.868	1.00	20.00
ATOM	1641	CG2	VAL	A	002	59.105	73.960	24.419	1.00	20.00
ATOM	1643	N	ARG	A	003	57.939	70.406	26.586	1.00	20.00
ATOM	1644	CA	ARG	A	003	57.158	69.637	27.519	1.00	20.00
ATOM	1645	C	ARG	A	003	57.966	68.497	28.085	1.00	20.00
ATOM	1646	O	ARG	A	003	57.686	68.013	29.163	1.00	20.00
ATOM	1647	CB	ARG	A	003	55.943	69.145	26.797	1.00	20.00
ATOM	1648	CG	ARG	A	003	55.600	70.041	25.655	1.00	20.00
ATOM	1649	CD	ARG	A	003	54.176	69.825	25.386	1.00	20.00
ATOM	1650	NE	ARG	A	003	53.404	70.556	26.347	1.00	20.00
ATOM	1651	CZ	ARG	A	003	52.340	71.236	25.991	1.00	20.00
ATOM	1652	NH1	ARG	A	003	52.002	71.218	24.710	1.00	20.00
ATOM	1653	NH2	ARG	A	003	51.653	71.922	26.889	1.00	20.00
ATOM	1660	N	TRP	A	004	58.998	68.136	27.340	1.00	20.00
ATOM	1661	CA	TRP	A	004	59.930	67.076	27.691	1.00	20.00
ATOM	1662	C	TRP	A	004	61.183	67.519	28.368	1.00	20.00
ATOM	1663	O	TRP	A	004	61.602	66.921	29.361	1.00	20.00
ATOM	1664	CB	TRP	A	004	60.293	66.257	26.452	1.00	20.00
ATOM	1665	CG	TRP	A	004	59.275	65.242	26.277	1.00	20.00
ATOM	1666	CD1	TRP	A	004	59.163	64.113	27.004	1.00	20.00
ATOM	1667	CD2	TRP	A	004	58.027	65.395	25.588	1.00	20.00
ATOM	1668	NE1	TRP	A	004	57.932	63.567	26.839	1.00	20.00
ATOM	1669	CE2	TRP	A	004	57.208	64.336	25.976	1.00	20.00
ATOM	1670	CE3	TRP	A	004	57.518	66.339	24.696	1.00	20.00
ATOM	1671	CZ2	TRP	A	004	55.911	64.185	25.506	1.00	20.00
ATOM	1672	CZ3	TRP	A	004	56.192	66.185	24.224	1.00	20.00
ATOM	1673	CH2	TRP	A	004	55.426	65.126	24.632	1.00	20.00
ATOM	1676	N	MET	A	005	61.767	68.590	27.874	1.00	20.00
ATOM	1677	CA	MET	A	005	63.025	69.060	28.428	1.00	20.00
ATOM	1678	C	MET	A	005	63.185	69.238	29.950	1.00	20.00
ATOM	1679	O	MET	A	005	62.268	69.013	30.733	1.00	20.00
ATOM	1680	CB	MET	A	005	63.433	70.335	27.699	1.00	20.00
ATOM	1681	CG	MET	A	005	64.246	70.052	26.452	1.00	20.00
ATOM	1682	SD	MET	A	005	63.856	71.198	25.171	1.00	20.00
ATOM	1683	CE	MET	A	005	64.138	72.700	26.081	1.00	20.00
ATOM	1685	N	ALA	A	006	64.402	69.581	30.358	1.00	20.00
ATOM	1686	CA	ALA	A	006	64.714	69.835	31.765	1.00	20.00

ATOM	1687	C	ALA	A	006	65.147	71.295	31.859	1.00	20.00
ATOM	1688	O	ALA	A	006	65.854	71.804	30.965	1.00	20.00
ATOM	1689	CB	ALA	A	006	65.819	68.944	32.215	1.00	20.00
ATOM	1691	N	ILE	A	007	64.694	71.961	32.930	1.00	20.00
ATOM	1692	CA	ILE	A	007	64.982	73.368	33.167	1.00	20.00
ATOM	1693	C	ILE	A	007	66.361	73.633	32.607	1.00	20.00
ATOM	1694	O	ILE	A	007	66.500	74.388	31.663	1.00	20.00
ATOM	1695	CB	ILE	A	007	64.876	73.725	34.674	1.00	20.00
ATOM	1696	CG1	ILE	A	007	65.897	72.943	35.501	1.00	20.00
ATOM	1697	CG2	ILE	A	007	63.518	73.339	35.193	1.00	20.00
ATOM	1698	CD1	ILE	A	007	66.781	73.773	36.516	1.00	20.00
ATOM	1700	N	GLU	A	008	67.361	72.921	33.131	1.00	20.00
ATOM	1701	CA	GLU	A	008	68.768	73.052	32.719	1.00	20.00
ATOM	1702	C	GLU	A	008	68.886	73.301	31.217	1.00	20.00
ATOM	1703	O	GLU	A	008	69.401	74.319	30.811	1.00	20.00
ATOM	1704	CB	GLU	A	008	69.565	71.799	33.174	1.00	20.00
ATOM	1705	CG	GLU	A	008	69.424	70.540	32.296	1.00	20.00
ATOM	1706	CD	GLU	A	008	69.290	69.267	33.131	1.00	20.00
ATOM	1707	OE1	GLU	A	008	69.605	69.369	34.325	1.00	20.00
ATOM	1708	OE2	GLU	A	008	68.867	68.187	32.613	1.00	20.00
ATOM	1710	N	SER	A	009	68.388	72.388	30.384	1.00	20.00
ATOM	1711	CA	SER	A	009	68.456	72.641	28.947	1.00	20.00
ATOM	1712	C	SER	A	009	67.387	73.630	28.440	1.00	20.00
ATOM	1713	O	SER	A	009	67.491	74.109	27.327	1.00	20.00
ATOM	1714	CB	SER	A	009	68.424	71.329	28.129	1.00	20.00
ATOM	1715	OG	SER	A	009	67.325	70.511	28.426	1.00	20.00
ATOM	1718	N	LEU	A	010	66.361	73.915	29.246	1.00	20.00
ATOM	1719	CA	LEU	A	010	65.328	74.909	28.869	1.00	20.00
ATOM	1720	C	LEU	A	010	66.043	76.294	28.797	1.00	20.00
ATOM	1721	O	LEU	A	010	65.881	77.047	27.816	1.00	20.00
ATOM	1722	CB	LEU	A	010	64.213	74.966	29.928	1.00	20.00
ATOM	1723	CG	LEU	A	010	62.880	74.229	29.760	1.00	20.00
ATOM	1724	CD1	LEU	A	010	61.863	75.034	30.483	1.00	20.00
ATOM	1725	CD2	LEU	A	010	62.459	74.066	28.330	1.00	20.00
ATOM	1727	N	ASN	A	011	66.825	76.577	29.854	1.00	20.00
ATOM	1728	CA	ASN	A	011	67.663	77.762	30.020	1.00	20.00
ATOM	1729	C	ASN	A	011	68.799	77.692	28.983	1.00	20.00
ATOM	1730	O	ASN	A	011	68.799	78.348	27.914	1.00	20.00
ATOM	1731	CB	ASN	A	011	68.303	77.725	31.386	1.00	20.00
ATOM	1732	CG	ASN	A	011	67.325	77.469	32.474	1.00	20.00
ATOM	1733	OD1	ASN	A	011	66.150	77.759	32.316	1.00	20.00
ATOM	1734	ND2	ASN	A	011	67.791	76.929	33.607	1.00	20.00
ATOM	1738	N	TYR	A	012	69.774	76.859	29.325	1.00	20.00
ATOM	1739	CA	TYR	A	012	70.918	76.611	28.481	1.00	20.00
ATOM	1740	C	TYR	A	012	70.488	75.487	27.544	1.00	20.00
ATOM	1741	O	TYR	A	012	69.908	74.499	28.020	1.00	20.00
ATOM	1742	CB	TYR	A	012	72.047	76.179	29.370	1.00	20.00
ATOM	1743	CG	TYR	A	012	71.787	76.590	30.784	1.00	20.00
ATOM	1744	CD1	TYR	A	012	71.854	75.680	31.809	1.00	20.00
ATOM	1745	CD2	TYR	A	012	71.474	77.879	31.097	1.00	20.00
ATOM	1746	CE1	TYR	A	012	71.619	76.047	33.097	1.00	20.00
ATOM	1747	CE2	TYR	A	012	71.246	78.242	32.357	1.00	20.00
ATOM	1748	CZ	TYR	A	012	71.321	77.328	33.361	1.00	20.00
ATOM	1749	OH	TYR	A	012	71.143	77.709	34.668	1.00	20.00
ATOM	1752	N	SER	A	013	70.711	75.615	26.235	1.00	20.00
ATOM	1753	CA	SER	A	013	70.309	74.544	25.335	1.00	20.00
ATOM	1754	C	SER	A	013	71.274	73.385	25.467	1.00	20.00

FIG. 4Y

ATOM	1755	O	SER	A	013	71.810	72.898	24.464	1.00	20.00
ATOM	1756	CB	SER	A	013	70.291	75.025	23.898	1.00	20.00
ATOM	1757	OG	SER	A	013	70.122	76.432	23.813	1.00	20.00
ATOM	1760	N	VAL	A	014	71.469	72.957	26.713	1.00	20.00
ATOM	1761	CA	VAL	A	014	72.378	71.890	27.084	1.00	20.00
ATOM	1762	C	VAL	A	014	71.711	70.603	27.571	1.00	20.00
ATOM	1763	O	VAL	A	014	70.895	70.613	28.493	1.00	20.00
ATOM	1764	CB	VAL	A	014	73.316	72.316	28.230	1.00	20.00
ATOM	1765	CG1	VAL	A	014	74.335	73.331	27.748	1.00	20.00
ATOM	1766	CG2	VAL	A	014	72.490	72.849	29.394	1.00	20.00
ATOM	1768	N	TYR	A	015	72.100	69.472	27.009	1.00	20.00
ATOM	1769	CA	TYR	A	015	71.502	68.235	27.446	1.00	20.00
ATOM	1770	C	TYR	A	015	72.543	67.266	28.029	1.00	20.00
ATOM	1771	O	TYR	A	015	73.619	67.072	27.494	1.00	20.00
ATOM	1772	CB	TYR	A	015	70.783	67.599	26.252	1.00	20.00
ATOM	1773	CG	TYR	A	015	69.875	68.533	25.477	1.00	20.00
ATOM	1774	CD1	TYR	A	015	70.194	68.918	24.179	1.00	20.00
ATOM	1775	CD2	TYR	A	015	68.665	68.975	26.022	1.00	20.00
ATOM	1776	CE1	TYR	A	015	69.334	69.718	23.416	1.00	20.00
ATOM	1777	CE2	TYR	A	015	67.782	69.778	25.286	1.00	20.00
ATOM	1778	CZ	TYR	A	015	68.116	70.150	23.968	1.00	20.00
ATOM	1779	OH	TYR	A	015	67.249	70.935	23.209	1.00	20.00
ATOM	1782	N	THR	A	016	72.253	66.679	29.161	1.00	20.00
ATOM	1783	CA	THR	A	016	73.172	65.695	29.673	1.00	20.00
ATOM	1784	C	THR	A	016	72.464	64.347	29.834	1.00	20.00
ATOM	1785	O	THR	A	016	71.573	63.995	29.086	1.00	20.00
ATOM	1786	CB	THR	A	016	73.717	66.097	31.000	1.00	20.00
ATOM	1787	OG1	THR	A	016	72.692	66.000	31.993	1.00	20.00
ATOM	1788	CG2	THR	A	016	74.253	67.455	30.909	1.00	20.00
ATOM	1791	N	THR	A	017	72.891	63.584	30.818	1.00	20.00
ATOM	1792	CA	THR	A	017	72.235	62.339	31.031	1.00	20.00
ATOM	1793	C	THR	A	017	71.021	62.785	31.819	1.00	20.00
ATOM	1794	O	THR	A	017	69.889	62.570	31.364	1.00	20.00
ATOM	1795	CB	THR	A	017	73.112	61.308	31.826	1.00	20.00
ATOM	1796	OG1	THR	A	017	73.546	60.286	30.931	1.00	20.00
ATOM	1797	CG2	THR	A	017	72.315	60.660	32.954	1.00	20.00
ATOM	1800	N	ASN	A	018	71.265	63.454	32.958	1.00	20.00
ATOM	1801	CA	ASN	A	018	70.189	63.934	33.825	1.00	20.00
ATOM	1802	C	ASN	A	018	69.025	64.568	33.108	1.00	20.00
ATOM	1803	O	ASN	A	018	67.937	64.530	33.636	1.00	20.00
ATOM	1804	CB	ASN	A	018	70.696	64.904	34.868	1.00	20.00
ATOM	1805	CG	ASN	A	018	71.785	64.331	35.676	1.00	20.00
ATOM	1806	OD1	ASN	A	018	71.761	64.412	36.887	1.00	20.00
ATOM	1807	ND2	ASN	A	018	72.767	63.734	35.013	1.00	20.00
ATOM	1811	N	SER	A	019	69.247	65.184	31.948	1.00	20.00
ATOM	1812	CA	SER	A	019	68.132	65.740	31.199	1.00	20.00
ATOM	1813	C	SER	A	019	67.362	64.513	30.704	1.00	20.00
ATOM	1814	O	SER	A	019	66.145	64.414	30.875	1.00	20.00
ATOM	1815	CB	SER	A	019	68.613	66.544	30.006	1.00	20.00
ATOM	1816	OG	SER	A	019	69.999	66.633	30.051	1.00	20.00
ATOM	1819	N	ASP	A	020	68.110	63.583	30.104	1.00	20.00
ATOM	1820	CA	ASP	A	020	67.596	62.309	29.604	1.00	20.00
ATOM	1821	C	ASP	A	020	66.784	61.679	30.741	1.00	20.00
ATOM	1822	O	ASP	A	020	65.672	61.194	30.543	1.00	20.00
ATOM	1823	CB	ASP	A	020	68.767	61.388	29.217	1.00	20.00
ATOM	1824	CG	ASP	A	020	69.154	61.484	27.729	1.00	20.00
ATOM	1825	OD1	ASP	A	020	68.649	62.363	26.979	1.00	20.00

FIG. 4Z

ATOM	1826	OD2	ASP	A	020	69.992	60.673	27.292	1.00	20.00
ATOM	1828	N	VAL	A	021	67.294	61.728	31.955	1.00	20.00
ATOM	1829	CA	VAL	A	021	66.522	61.083	32.960	1.00	20.00
ATOM	1830	C	VAL	A	021	65.300	61.826	33.326	1.00	20.00
ATOM	1831	O	VAL	A	021	64.372	61.212	33.879	1.00	20.00
ATOM	1832	CB	VAL	A	021	67.316	60.766	34.204	1.00	20.00
ATOM	1833	CG1	VAL	A	021	66.471	60.862	35.417	1.00	20.00
ATOM	1834	CG2	VAL	A	021	67.803	59.362	34.110	1.00	20.00
ATOM	1836	N	TRP	A	022	65.290	63.135	33.035	1.00	20.00
ATOM	1837	CA	TRP	A	022	64.157	64.016	33.326	1.00	20.00
ATOM	1838	C	TRP	A	022	63.051	63.699	32.319	1.00	20.00
ATOM	1839	O	TRP	A	022	61.948	63.268	32.629	1.00	20.00
ATOM	1840	CB	TRP	A	022	64.596	65.468	33.160	1.00	20.00
ATOM	1841	CG	TRP	A	022	63.439	66.467	33.254	1.00	20.00
ATOM	1842	CD1	TRP	A	022	62.437	66.648	32.337	1.00	20.00
ATOM	1843	CD2	TRP	A	022	63.161	67.366	34.322	1.00	20.00
ATOM	1844	NE1	TRP	A	022	61.576	67.578	32.767	1.00	20.00
ATOM	1845	CE2	TRP	A	022	61.985	68.049	33.984	1.00	20.00
ATOM	1846	CE3	TRP	A	022	63.791	67.662	35.529	1.00	20.00
ATOM	1847	CZ2	TRP	A	022	61.413	69.029	34.815	1.00	20.00
ATOM	1848	CZ3	TRP	A	022	63.237	68.626	36.355	1.00	20.00
ATOM	1849	CH2	TRP	A	022	62.052	69.303	35.992	1.00	20.00
ATOM	1852	N	SER	A	023	63.407	63.969	31.084	1.00	20.00
ATOM	1853	CA	SER	A	023	62.591	63.721	29.928	1.00	20.00
ATOM	1854	C	SER	A	023	61.978	62.316	30.007	1.00	20.00
ATOM	1855	O	SER	A	023	60.863	62.092	29.540	1.00	20.00
ATOM	1856	CB	SER	A	023	63.497	63.860	28.709	1.00	20.00
ATOM	1857	OG	SER	A	023	62.747	63.795	27.527	1.00	20.00
ATOM	1860	N	TYR	A	024	62.731	61.390	30.617	1.00	20.00
ATOM	1861	CA	TYR	A	024	62.361	59.980	30.801	1.00	20.00
ATOM	1862	C	TYR	A	024	60.980	59.761	31.454	1.00	20.00
ATOM	1863	O	TYR	A	024	60.137	58.991	30.967	1.00	20.00
ATOM	1864	CB	TYR	A	024	63.436	59.307	31.627	1.00	20.00
ATOM	1865	CG	TYR	A	024	63.129	57.866	31.859	1.00	20.00
ATOM	1866	CD1	TYR	A	024	63.276	56.948	30.849	1.00	20.00
ATOM	1867	CD2	TYR	A	024	62.479	57.473	33.019	1.00	20.00
ATOM	1868	CE1	TYR	A	024	62.766	55.706	30.979	1.00	20.00
ATOM	1869	CE2	TYR	A	024	61.962	56.236	33.157	1.00	20.00
ATOM	1870	CZ	TYR	A	024	62.099	55.365	32.135	1.00	20.00
ATOM	1871	OH	TYR	A	024	61.517	54.160	32.263	1.00	20.00
ATOM	1874	N	GLY	A	025	60.803	60.436	32.583	1.00	20.00
ATOM	1875	CA	GLY	A	025	59.558	60.427	33.311	1.00	20.00
ATOM	1876	C	GLY	A	025	58.477	61.257	32.614	1.00	20.00
ATOM	1877	O	GLY	A	025	57.365	61.290	33.058	1.00	20.00
ATOM	1879	N	VAL	A	026	58.747	61.974	31.544	1.00	20.00
ATOM	1880	CA	VAL	A	026	57.596	62.614	30.980	1.00	20.00
ATOM	1881	C	VAL	A	026	57.057	61.313	30.484	1.00	20.00
ATOM	1882	O	VAL	A	026	56.006	60.906	30.923	1.00	20.00
ATOM	1883	CB	VAL	A	026	57.889	63.625	29.823	1.00	20.00
ATOM	1884	CG1	VAL	A	026	56.583	64.258	29.328	1.00	20.00
ATOM	1885	CG2	VAL	A	026	58.746	64.717	30.327	1.00	20.00
ATOM	1887	N	LEU	A	027	57.843	60.639	29.632	1.00	20.00
ATOM	1888	CA	LEU	A	027	57.535	59.273	29.064	1.00	20.00
ATOM	1889	C	LEU	A	027	56.767	58.278	30.014	1.00	20.00
ATOM	1890	O	LEU	A	027	55.745	57.736	29.702	1.00	20.00
ATOM	1891	CB	LEU	A	027	58.852	58.615	28.663	1.00	20.00
ATOM	1892	CG	LEU	A	027	58.843	57.551	27.579	1.00	20.00

FIG. 4AA

ATOM	1893	CD1	LEU	A	027	58.238	58.171	26.367	1.00	20.00
ATOM	1894	CD2	LEU	A	027	60.239	57.031	27.287	1.00	20.00
ATOM	1896	N	LEU	A	028	57.333	58.031	31.171	1.00	20.00
ATOM	1897	CA	LEU	A	028	56.723	57.188	32.128	1.00	20.00
ATOM	1898	C	LEU	A	028	55.330	57.638	32.349	1.00	20.00
ATOM	1899	O	LEU	A	028	54.428	56.817	32.517	1.00	20.00
ATOM	1900	CB	LEU	A	028	57.455	57.281	33.427	1.00	20.00
ATOM	1901	CG	LEU	A	028	56.778	56.395	34.430	1.00	20.00
ATOM	1902	CD1	LEU	A	028	56.765	55.005	33.926	1.00	20.00
ATOM	1903	CD2	LEU	A	028	57.488	56.475	35.740	1.00	20.00
ATOM	1905	N	TRP	A	029	55.148	58.961	32.409	1.00	20.00
ATOM	1906	CA	TRP	A	029	53.820	59.578	32.612	1.00	20.00
ATOM	1907	C	TRP	A	029	53.028	59.464	31.295	1.00	20.00
ATOM	1908	O	TRP	A	029	51.869	59.142	31.301	1.00	20.00
ATOM	1909	CB	TRP	A	029	54.010	61.029	33.088	1.00	20.00
ATOM	1910	CG	TRP	A	029	52.746	61.841	33.293	1.00	20.00
ATOM	1911	CD1	TRP	A	029	52.207	62.275	34.483	1.00	20.00
ATOM	1912	CD2	TRP	A	029	51.934	62.381	32.271	1.00	20.00
ATOM	1913	NE1	TRP	A	029	51.113	63.057	34.241	1.00	20.00
ATOM	1914	CE2	TRP	A	029	50.925	63.138	32.892	1.00	20.00
ATOM	1915	CE3	TRP	A	029	51.962	62.298	30.886	1.00	20.00
ATOM	1916	CZ2	TRP	A	029	49.975	63.798	32.185	1.00	20.00
ATOM	1917	CZ3	TRP	A	029	51.018	62.951	30.186	1.00	20.00
ATOM	1918	CH2	TRP	A	029	50.030	63.701	30.830	1.00	20.00
ATOM	1921	N	GLU	A	030	53.684	59.695	30.166	1.00	20.00
ATOM	1922	CA	GLU	A	030	53.067	59.537	28.861	1.00	20.00
ATOM	1923	C	GLU	A	030	52.592	58.103	28.823	1.00	20.00
ATOM	1924	O	GLU	A	030	51.775	57.758	27.982	1.00	20.00
ATOM	1925	CB	GLU	A	030	54.099	59.616	27.737	1.00	20.00
ATOM	1926	CG	GLU	A	030	54.380	60.917	27.071	1.00	20.00
ATOM	1927	CD	GLU	A	030	55.162	60.706	25.771	1.00	20.00
ATOM	1928	OE1	GLU	A	030	55.818	59.668	25.665	1.00	20.00
ATOM	1929	OE2	GLU	A	030	55.144	61.535	24.838	1.00	20.00
ATOM	1931	N	ILE	A	031	53.124	57.260	29.711	1.00	20.00
ATOM	1932	CA	ILE	A	031	52.839	55.820	29.680	1.00	20.00
ATOM	1933	C	ILE	A	031	51.803	55.305	30.628	1.00	20.00
ATOM	1934	O	ILE	A	031	50.931	54.585	30.219	1.00	20.00
ATOM	1935	CB	ILE	A	031	54.192	54.974	29.833	1.00	20.00
ATOM	1936	CG1	ILE	A	031	54.803	54.722	28.459	1.00	20.00
ATOM	1937	CG2	ILE	A	031	53.964	53.607	30.495	1.00	20.00
ATOM	1938	CD1	ILE	A	031	56.144	54.104	28.543	1.00	20.00
ATOM	1940	N	VAL	A	032	51.893	55.672	31.892	1.00	20.00
ATOM	1941	CA	VAL	A	032	50.918	55.223	32.895	1.00	20.00
ATOM	1942	C	VAL	A	032	49.618	55.914	32.620	1.00	20.00
ATOM	1943	O	VAL	A	032	48.706	55.811	33.412	1.00	20.00
ATOM	1944	CB	VAL	A	032	51.306	55.664	34.327	1.00	20.00
ATOM	1945	CG1	VAL	A	032	50.610	56.932	34.667	1.00	20.00
ATOM	1946	CG2	VAL	A	032	50.962	54.602	35.333	1.00	20.00
ATOM	1948	N	SER	A	033	49.552	56.605	31.493	1.00	20.00
ATOM	1949	CA	SER	A	033	48.413	57.405	31.146	1.00	20.00
ATOM	1950	C	SER	A	033	47.776	57.027	29.850	1.00	20.00
ATOM	1951	O	SER	A	033	46.634	57.396	29.585	1.00	20.00
ATOM	1952	CB	SER	A	033	48.828	58.889	31.116	1.00	20.00
ATOM	1953	OG	SER	A	033	49.492	59.239	29.905	1.00	20.00
ATOM	1956	N	LEU	A	034	48.513	56.329	29.019	1.00	20.00
ATOM	1957	CA	LEU	A	034	47.975	55.904	27.758	1.00	20.00
ATOM	1958	C	LEU	A	034	47.939	57.037	26.801	1.00	20.00

FIG. 4BB

ATOM	1959	O	LEU	A	034	46.917	57.357	26.219	1.00	20.00
ATOM	1960	CB	LEU	A	034	46.580	55.366	27.923	1.00	20.00
ATOM	1961	CG	LEU	A	034	46.208	54.020	28.500	1.00	20.00
ATOM	1962	CD1	LEU	A	034	46.074	54.041	29.977	1.00	20.00
ATOM	1963	CD2	LEU	A	034	44.892	53.709	27.900	1.00	20.00
ATOM	1965	N	GLY	A	035	49.091	57.663	26.658	1.00	20.00
ATOM	1966	CA	GLY	A	035	49.248	58.759	25.715	1.00	20.00
ATOM	1967	C	GLY	A	035	48.581	60.112	25.920	1.00	20.00
ATOM	1968	O	GLY	A	035	48.145	60.734	24.947	1.00	20.00
ATOM	1970	N	GLY	A	036	48.511	60.580	27.156	1.00	20.00
ATOM	1971	CA	GLY	A	036	47.902	61.874	27.364	1.00	20.00
ATOM	1972	C	GLY	A	036	48.981	62.925	27.245	1.00	20.00
ATOM	1973	O	GLY	A	036	50.097	62.697	27.759	1.00	20.00
ATOM	1975	N	THR	A	037	48.692	64.027	26.543	1.00	20.00
ATOM	1976	CA	THR	A	037	49.656	65.126	26.400	1.00	20.00
ATOM	1977	C	THR	A	037	50.114	65.691	27.757	1.00	20.00
ATOM	1978	O	THR	A	037	49.289	65.966	28.616	1.00	20.00
ATOM	1979	CB	THR	A	037	49.038	66.308	25.664	1.00	20.00
ATOM	1980	OG1	THR	A	037	49.457	66.326	24.301	1.00	20.00
ATOM	1981	CG2	THR	A	037	49.447	67.597	26.327	1.00	20.00
ATOM	1984	N	PRO	A	038	51.445	65.866	27.966	1.00	20.00
ATOM	1985	CA	PRO	A	038	51.925	66.416	29.237	1.00	20.00
ATOM	1986	C	PRO	A	038	51.674	67.919	29.265	1.00	20.00
ATOM	1987	O	PRO	A	038	51.812	68.570	28.264	1.00	20.00
ATOM	1988	CB	PRO	A	038	53.401	66.083	29.223	1.00	20.00
ATOM	1989	CG	PRO	A	038	53.573	65.116	28.170	1.00	20.00
ATOM	1990	CD	PRO	A	038	52.592	65.497	27.134	1.00	20.00
ATOM	1991	N	TYR	A	039	51.296	68.471	30.407	1.00	20.00
ATOM	1992	CA	TYR	A	039	51.040	69.900	30.494	1.00	20.00
ATOM	1993	C	TYR	A	039	49.928	70.255	29.514	1.00	20.00
ATOM	1994	O	TYR	A	039	50.174	71.011	28.551	1.00	20.00
ATOM	1995	CB	TYR	A	039	52.317	70.678	30.156	1.00	20.00
ATOM	1996	CG	TYR	A	039	53.492	70.254	31.016	1.00	20.00
ATOM	1997	CD1	TYR	A	039	54.593	69.571	30.470	1.00	20.00
ATOM	1998	CD2	TYR	A	039	53.456	70.437	32.381	1.00	20.00
ATOM	1999	CE1	TYR	A	039	55.586	69.088	31.288	1.00	20.00
ATOM	2000	CE2	TYR	A	039	54.438	69.966	33.188	1.00	20.00
ATOM	2001	CZ	TYR	A	039	55.489	69.290	32.656	1.00	20.00
ATOM	2002	OH	TYR	A	039	56.405	68.759	33.532	1.00	20.00
ATOM	2005	N	CYS	A	040	48.713	69.706	29.757	1.00	20.00
ATOM	2006	CA	CYS	A	040	47.536	69.943	28.893	1.00	20.00
ATOM	2007	C	CYS	A	040	46.861	71.241	29.251	1.00	20.00
ATOM	2008	O	CYS	A	040	46.426	71.456	30.371	1.00	20.00
ATOM	2009	CB	CYS	A	040	46.518	68.779	28.952	1.00	20.00
ATOM	2010	SG	CYS	A	040	45.587	68.439	27.332	1.00	20.00
ATOM	2012	N	GLY	A	041	46.773	72.105	28.261	1.00	20.00
ATOM	2013	CA	GLY	A	041	46.197	73.417	28.496	1.00	20.00
ATOM	2014	C	GLY	A	041	47.251	74.257	29.222	1.00	20.00
ATOM	2015	O	GLY	A	041	46.977	74.928	30.241	1.00	20.00
ATOM	2017	N	MET	A	042	48.480	74.184	28.727	1.00	20.00
ATOM	2018	CA	MET	A	042	49.542	74.920	29.347	1.00	20.00
ATOM	2019	C	MET	A	042	50.391	75.508	28.241	1.00	20.00
ATOM	2020	O	MET	A	042	50.540	74.944	27.173	1.00	20.00
ATOM	2021	CB	MET	A	042	50.321	73.990	30.253	1.00	20.00
ATOM	2022	CG	MET	A	042	50.038	74.150	31.721	1.00	20.00
ATOM	2023	SD	MET	A	042	51.637	74.393	32.551	1.00	20.00
ATOM	2024	CE	MET	A	042	51.370	73.664	34.142	1.00	20.00

FIG. 4CC

ATOM	2026	N	THR	A	043	50.915	76.686	28.463	1.00	20.00
ATOM	2027	CA	THR	A	043	51.699	77.320	27.418	1.00	20.00
ATOM	2028	C	THR	A	043	53.137	77.204	27.856	1.00	20.00
ATOM	2029	O	THR	A	043	53.479	77.409	29.047	1.00	20.00
ATOM	2030	CB	THR	A	043	51.356	78.827	27.279	1.00	20.00
ATOM	2031	OG1	THR	A	043	51.534	79.465	28.565	1.00	20.00
ATOM	2032	CG2	THR	A	043	49.905	79.033	26.760	1.00	20.00
ATOM	2035	N	CYS	A	044	53.977	76.852	26.885	1.00	20.00
ATOM	2036	CA	CYS	A	044	55.388	76.714	27.139	1.00	20.00
ATOM	2037	C	CYS	A	044	55.681	77.866	28.075	1.00	20.00
ATOM	2038	O	CYS	A	044	55.836	77.638	29.269	1.00	20.00
ATOM	2039	CB	CYS	A	044	56.128	76.779	25.814	1.00	20.00
ATOM	2040	SG	CYS	A	044	55.373	75.549	24.616	1.00	20.00
ATOM	2042	N	ALA	A	045	55.664	79.092	27.554	1.00	20.00
ATOM	2043	CA	ALA	A	045	55.893	80.306	28.342	1.00	20.00
ATOM	2044	C	ALA	A	045	55.536	80.155	29.809	1.00	20.00
ATOM	2045	O	ALA	A	045	56.216	80.636	30.700	1.00	20.00
ATOM	2046	CB	ALA	A	045	55.082	81.416	27.760	1.00	20.00
ATOM	2048	N	GLU	A	046	54.429	79.482	30.050	1.00	20.00
ATOM	2049	CA	GLU	A	046	53.961	79.269	31.390	1.00	20.00
ATOM	2050	C	GLU	A	046	54.902	78.299	32.100	1.00	20.00
ATOM	2051	O	GLU	A	046	55.309	78.558	33.243	1.00	20.00
ATOM	2052	CB	GLU	A	046	52.556	78.738	31.281	1.00	20.00
ATOM	2053	CG	GLU	A	046	51.601	79.002	32.429	1.00	20.00
ATOM	2054	CD	GLU	A	046	50.437	78.036	32.341	1.00	20.00
ATOM	2055	OE1	GLU	A	046	50.182	77.380	33.378	1.00	20.00
ATOM	2056	OE2	GLU	A	046	49.814	77.940	31.222	1.00	20.00
ATOM	2058	N	LEU	A	047	55.251	77.192	31.437	1.00	20.00
ATOM	2059	CA	LEU	A	047	56.203	76.207	32.001	1.00	20.00
ATOM	2060	C	LEU	A	047	57.470	76.893	32.593	1.00	20.00
ATOM	2061	O	LEU	A	047	57.712	76.853	33.805	1.00	20.00
ATOM	2062	CB	LEU	A	047	56.639	75.203	30.914	1.00	20.00
ATOM	2063	CG	LEU	A	047	55.895	73.858	30.885	1.00	20.00
ATOM	2064	CD1	LEU	A	047	56.520	72.889	29.922	1.00	20.00
ATOM	2065	CD2	LEU	A	047	55.884	73.280	32.256	1.00	20.00
ATOM	2067	N	TYR	A	048	58.254	77.503	31.694	1.00	20.00
ATOM	2068	CA	TYR	A	048	59.483	78.267	31.974	1.00	20.00
ATOM	2069	C	TYR	A	048	59.499	78.978	33.311	1.00	20.00
ATOM	2070	O	TYR	A	048	60.325	78.669	34.188	1.00	20.00
ATOM	2071	CB	TYR	A	048	59.684	79.343	30.919	1.00	20.00
ATOM	2072	CG	TYR	A	048	60.217	78.874	29.611	1.00	20.00
ATOM	2073	CD1	TYR	A	048	59.370	78.692	28.518	1.00	20.00
ATOM	2074	CD2	TYR	A	048	61.570	78.629	29.459	1.00	20.00
ATOM	2075	CE1	TYR	A	048	59.868	78.263	27.278	1.00	20.00
ATOM	2076	CE2	TYR	A	048	62.094	78.206	28.248	1.00	20.00
ATOM	2077	CZ	TYR	A	048	61.250	78.013	27.141	1.00	20.00
ATOM	2078	OH	TYR	A	048	61.799	77.541	25.930	1.00	20.00
ATOM	2081	N	GLU	A	049	58.601	79.954	33.446	1.00	20.00
ATOM	2082	CA	GLU	A	049	58.527	80.725	34.680	1.00	20.00
ATOM	2083	C	GLU	A	049	58.074	79.756	35.720	1.00	20.00
ATOM	2084	O	GLU	A	049	58.417	79.886	36.903	1.00	20.00
ATOM	2085	CB	GLU	A	049	57.485	81.840	34.592	1.00	20.00
ATOM	2086	CG	GLU	A	049	57.233	82.519	35.947	1.00	20.00
ATOM	2087	CD	GLU	A	049	55.761	82.820	36.314	1.00	20.00
ATOM	2088	OE1	GLU	A	049	54.860	82.700	35.453	1.00	20.00
ATOM	2089	OE2	GLU	A	049	55.540	83.185	37.497	1.00	20.00
ATOM	2091	N	LYS	A	050	57.277	78.791	35.243	1.00	20.00

FIG. 4DD

ATOM	2092	CA	LYS	A	050	56.683	77.749	36.092	1.00	20.00
ATOM	2093	C	LYS	A	050	57.625	76.655	36.652	1.00	20.00
ATOM	2094	O	LYS	A	050	58.038	76.747	37.789	1.00	20.00
ATOM	2095	CB	LYS	A	050	55.465	77.116	35.362	1.00	20.00
ATOM	2097	N	LEU	A	051	57.965	75.640	35.880	1.00	20.00
ATOM	2098	CA	LEU	A	051	58.854	74.592	36.398	1.00	20.00
ATOM	2099	C	LEU	A	051	59.828	75.002	37.553	1.00	20.00
ATOM	2100	O	LEU	A	051	59.835	74.350	38.608	1.00	20.00
ATOM	2101	CB	LEU	A	051	59.655	73.957	35.239	1.00	20.00
ATOM	2102	CG	LEU	A	051	58.981	72.988	34.248	1.00	20.00
ATOM	2103	CD1	LEU	A	051	57.669	72.566	34.798	1.00	20.00
ATOM	2104	CD2	LEU	A	051	58.796	73.609	32.875	1.00	20.00
ATOM	2106	N	PRO	A	052	60.673	76.050	37.346	1.00	20.00
ATOM	2107	CA	PRO	A	052	61.652	76.601	38.292	1.00	20.00
ATOM	2108	C	PRO	A	052	61.323	76.418	39.750	1.00	20.00
ATOM	2109	O	PRO	A	052	61.675	75.396	40.337	1.00	20.00
ATOM	2110	CB	PRO	A	052	61.724	78.053	37.895	1.00	20.00
ATOM	2111	CG	PRO	A	052	61.556	78.008	36.389	1.00	20.00
ATOM	2112	CD	PRO	A	052	60.771	76.762	36.051	1.00	20.00
ATOM	2113	N	GLN	A	053	60.706	77.399	40.394	1.00	20.00
ATOM	2114	CA	GLN	A	053	60.319	77.126	41.783	1.00	20.00
ATOM	2115	C	GLN	A	053	58.915	76.531	41.498	1.00	20.00
ATOM	2116	O	GLN	A	053	58.116	76.198	42.386	1.00	20.00
ATOM	2117	CB	GLN	A	053	60.274	78.414	42.664	1.00	20.00
ATOM	2119	N	GLY	A	054	58.649	76.413	40.208	1.00	20.00
ATOM	2120	CA	GLY	A	054	57.454	75.745	39.784	1.00	20.00
ATOM	2121	C	GLY	A	054	57.520	74.261	40.190	1.00	20.00
ATOM	2122	O	GLY	A	054	58.564	73.730	40.654	1.00	20.00
ATOM	2124	N	TYR	A	055	56.363	73.629	40.002	1.00	20.00
ATOM	2125	CA	TYR	A	055	56.081	72.268	40.370	1.00	20.00
ATOM	2126	C	TYR	A	055	56.216	71.476	39.095	1.00	20.00
ATOM	2127	O	TYR	A	055	56.762	72.008	38.153	1.00	20.00
ATOM	2128	CB	TYR	A	055	54.647	72.256	40.889	1.00	20.00
ATOM	2129	CG	TYR	A	055	53.604	72.330	39.754	1.00	20.00
ATOM	2130	CD1	TYR	A	055	52.634	71.309	39.604	1.00	20.00
ATOM	2131	CD2	TYR	A	055	53.685	73.316	38.749	1.00	20.00
ATOM	2132	CE1	TYR	A	055	51.805	71.283	38.478	1.00	20.00
ATOM	2133	CE2	TYR	A	055	52.863	73.280	37.642	1.00	20.00
ATOM	2134	CZ	TYR	A	055	51.928	72.264	37.501	1.00	20.00
ATOM	2135	OH	TYR	A	055	51.114	72.171	36.375	1.00	20.00
ATOM	2138	N	ARG	A	056	55.738	70.232	39.048	1.00	20.00
ATOM	2139	CA	ARG	A	056	55.828	69.422	37.821	1.00	20.00
ATOM	2140	C	ARG	A	056	54.504	68.699	37.494	1.00	20.00
ATOM	2141	O	ARG	A	056	53.471	69.052	38.098	1.00	20.00
ATOM	2142	CB	ARG	A	056	56.926	68.379	37.948	1.00	20.00
ATOM	2143	CG	ARG	A	056	57.175	67.962	39.357	1.00	20.00
ATOM	2144	CD	ARG	A	056	58.538	68.505	39.833	1.00	20.00
ATOM	2145	NE	ARG	A	056	59.319	69.142	38.760	1.00	20.00
ATOM	2146	CZ	ARG	A	056	60.182	70.114	38.982	1.00	20.00
ATOM	2147	NH1	ARG	A	056	60.367	70.542	40.201	1.00	20.00
ATOM	2148	NH2	ARG	A	056	60.839	70.655	37.996	1.00	20.00
ATOM	2155	N	LEU	A	057	54.531	67.705	36.565	1.00	20.00
ATOM	2156	CA	LEU	A	057	53.312	66.955	36.203	1.00	20.00
ATOM	2157	C	LEU	A	057	52.643	66.257	37.370	1.00	20.00
ATOM	2158	O	LEU	A	057	53.221	65.587	38.191	1.00	20.00
ATOM	2159	CB	LEU	A	057	53.519	65.955	35.071	1.00	20.00
ATOM	2160	CG	LEU	A	057	53.850	66.384	33.632	1.00	20.00

FIG. 4EE

ATOM	2161	CD1	LEU	A	057	54.504	65.224	32.920	1.00	20.00
ATOM	2162	CD2	LEU	A	057	52.669	66.811	32.830	1.00	20.00
ATOM	2164	N	GLU	A	058	51.357	66.515	37.390	1.00	20.00
ATOM	2165	CA	GLU	A	058	50.325	66.093	38.333	1.00	20.00
ATOM	2166	C	GLU	A	058	50.078	64.562	38.297	1.00	20.00
ATOM	2167	O	GLU	A	058	50.013	63.978	37.216	1.00	20.00
ATOM	2168	CB	GLU	A	058	49.091	66.872	37.885	1.00	20.00
ATOM	2169	CG	GLU	A	058	48.798	66.637	36.334	1.00	20.00
ATOM	2170	CD	GLU	A	058	49.565	67.548	35.341	1.00	20.00
ATOM	2171	OE1	GLU	A	058	50.058	68.604	35.777	1.00	20.00
ATOM	2172	OE2	GLU	A	058	49.657	67.227	34.128	1.00	20.00
ATOM	2174	N	LYS	A	059	49.906	63.915	39.448	1.00	20.00
ATOM	2175	CA	LYS	A	059	49.693	62.458	39.420	1.00	20.00
ATOM	2176	C	LYS	A	059	48.502	61.929	38.655	1.00	20.00
ATOM	2177	O	LYS	A	059	47.366	62.213	38.971	1.00	20.00
ATOM	2178	CB	LYS	A	059	49.607	61.825	40.814	1.00	20.00
ATOM	2179	CG	LYS	A	059	49.383	60.289	40.717	1.00	20.00
ATOM	2180	CD	LYS	A	059	49.519	59.551	42.056	1.00	20.00
ATOM	2181	CE	LYS	A	059	48.286	59.754	42.979	1.00	20.00
ATOM	2182	NZ	LYS	A	059	47.400	58.540	43.161	1.00	20.00
ATOM	2187	N	PRO	A	060	48.753	61.095	37.662	1.00	20.00
ATOM	2188	CA	PRO	A	060	47.615	60.576	36.931	1.00	20.00
ATOM	2189	C	PRO	A	060	46.646	59.848	37.873	1.00	20.00
ATOM	2190	O	PRO	A	060	47.048	59.234	38.860	1.00	20.00
ATOM	2191	CB	PRO	A	060	48.260	59.643	35.923	1.00	20.00
ATOM	2192	CG	PRO	A	060	49.662	60.187	35.751	1.00	20.00
ATOM	2193	CD	PRO	A	060	50.018	60.555	37.147	1.00	20.00
ATOM	2194	N	LEU	A	061	45.371	59.984	37.543	1.00	20.00
ATOM	2195	CA	LEU	A	061	44.236	59.426	38.245	1.00	20.00
ATOM	2196	C	LEU	A	061	44.496	58.098	38.924	1.00	20.00
ATOM	2197	O	LEU	A	061	44.187	57.890	40.123	1.00	20.00
ATOM	2198	CB	LEU	A	061	43.055	59.243	37.248	1.00	20.00
ATOM	2199	CG	LEU	A	061	42.994	59.507	35.690	1.00	20.00
ATOM	2200	CD1	LEU	A	061	44.393	59.876	35.050	1.00	20.00
ATOM	2201	CD2	LEU	A	061	42.384	58.237	35.000	1.00	20.00
ATOM	2203	N	ASN	A	062	45.075	57.203	38.117	1.00	20.00
ATOM	2204	CA	ASN	A	062	45.378	55.820	38.502	1.00	20.00
ATOM	2205	C	ASN	A	062	46.840	55.286	38.537	1.00	20.00
ATOM	2206	O	ASN	A	062	47.079	54.209	37.999	1.00	20.00
ATOM	2207	CB	ASN	A	062	44.591	54.958	37.559	1.00	20.00
ATOM	2208	CG	ASN	A	062	44.675	55.478	36.220	1.00	20.00
ATOM	2209	OD1	ASN	A	062	45.731	55.960	35.816	1.00	20.00
ATOM	2210	ND2	ASN	A	062	43.590	55.443	35.504	1.00	20.00
ATOM	2214	N	CYS	A	063	47.812	56.005	39.100	1.00	20.00
ATOM	2215	CA	CYS	A	063	49.165	55.418	39.205	1.00	20.00
ATOM	2216	C	CYS	A	063	49.155	55.124	40.645	1.00	20.00
ATOM	2217	O	CYS	A	063	48.285	55.550	41.377	1.00	20.00
ATOM	2218	CB	CYS	A	063	50.364	56.362	39.046	1.00	20.00
ATOM	2219	SG	CYS	A	063	50.817	56.807	37.453	1.00	20.00
ATOM	2221	N	ASP	A	064	50.186	54.449	41.067	1.00	20.00
ATOM	2222	CA	ASP	A	064	50.291	54.106	42.448	1.00	20.00
ATOM	2223	C	ASP	A	064	51.455	54.945	42.917	1.00	20.00
ATOM	2224	O	ASP	A	064	52.521	54.903	42.319	1.00	20.00
ATOM	2225	CB	ASP	A	064	50.558	52.601	42.552	1.00	20.00
ATOM	2226	CG	ASP	A	064	50.951	52.180	43.945	1.00	20.00
ATOM	2227	OD1	ASP	A	064	50.078	51.628	44.664	1.00	20.00
ATOM	2228	OD2	ASP	A	064	52.131	52.394	44.309	1.00	20.00

FIG. 4FF

ATOM	2230	N	ASP A 065	51.259	55.718	43.973	1.00	20.00
ATOM	2231	CA	ASP A 065	52.332	56.577	44.460	1.00	20.00
ATOM	2232	C	ASP A 065	53.733	56.051	44.341	1.00	20.00
ATOM	2233	O	ASP A 065	54.642	56.860	44.332	1.00	20.00
ATOM	2234	CB	ASP A 065	52.062	57.029	45.875	1.00	20.00
ATOM	2235	CG	ASP A 065	50.937	58.020	45.923	1.00	20.00
ATOM	2236	OD1	ASP A 065	50.842	58.814	44.958	1.00	20.00
ATOM	2237	OD2	ASP A 065	50.136	58.013	46.883	1.00	20.00
ATOM	2239	N	GLU A 066	53.918	54.734	44.222	1.00	20.00
ATOM	2240	CA	GLU A 066	55.255	54.179	44.049	1.00	20.00
ATOM	2241	C	GLU A 066	55.670	54.466	42.600	1.00	20.00
ATOM	2242	O	GLU A 066	56.854	54.554	42.311	1.00	20.00
ATOM	2243	CB	GLU A 066	55.315	52.656	44.363	1.00	20.00
ATOM	2244	CG	GLU A 066	54.520	52.182	45.635	1.00	20.00
ATOM	2245	CD	GLU A 066	54.944	50.804	46.237	1.00	20.00
ATOM	2246	OE1	GLU A 066	54.716	50.604	47.469	1.00	20.00
ATOM	2247	OE2	GLU A 066	55.494	49.937	45.496	1.00	20.00
ATOM	2249	N	VAL A 067	54.726	54.592	41.671	1.00	20.00
ATOM	2250	CA	VAL A 067	55.092	54.941	40.293	1.00	20.00
ATOM	2251	C	VAL A 067	55.224	56.462	40.180	1.00	20.00
ATOM	2252	O	VAL A 067	56.000	56.986	39.410	1.00	20.00
ATOM	2253	CB	VAL A 067	54.055	54.487	39.279	1.00	20.00
ATOM	2254	CG1	VAL A 067	54.600	54.593	37.857	1.00	20.00
ATOM	2255	CG2	VAL A 067	53.657	53.116	39.597	1.00	20.00
ATOM	2257	N	TYR A 068	54.460	57.189	40.948	1.00	20.00
ATOM	2258	CA	TYR A 068	54.614	58.609	40.861	1.00	20.00
ATOM	2259	C	TYR A 068	55.973	59.018	41.455	1.00	20.00
ATOM	2260	O	TYR A 068	56.712	59.819	40.831	1.00	20.00
ATOM	2261	CB	TYR A 068	53.489	59.313	41.595	1.00	20.00
ATOM	2262	CG	TYR A 068	53.361	60.752	41.220	1.00	20.00
ATOM	2263	CD1	TYR A 068	53.128	61.124	39.920	1.00	20.00
ATOM	2264	CD2	TYR A 068	53.490	61.746	42.186	1.00	20.00
ATOM	2265	CE1	TYR A 068	53.031	62.478	39.603	1.00	20.00
ATOM	2266	CE2	TYR A 068	53.395	63.060	41.887	1.00	20.00
ATOM	2267	CZ	TYR A 068	53.171	63.435	40.612	1.00	20.00
ATOM	2268	OH	TYR A 068	53.121	64.768	40.328	1.00	20.00
ATOM	2271	N	ASP A 069	56.315	58.503	42.647	1.00	20.00
ATOM	2272	CA	ASP A 069	57.609	58.859	43.214	1.00	20.00
ATOM	2273	C	ASP A 069	58.773	58.615	42.263	1.00	20.00
ATOM	2274	O	ASP A 069	59.744	59.344	42.299	1.00	20.00
ATOM	2275	CB	ASP A 069	57.969	58.107	44.464	1.00	20.00
ATOM	2276	CG	ASP A 069	59.422	58.423	44.879	1.00	20.00
ATOM	2277	OD1	ASP A 069	60.352	57.615	44.540	1.00	20.00
ATOM	2278	OD2	ASP A 069	59.635	59.510	45.509	1.00	20.00
ATOM	2280	N	LEU A 070	58.720	57.565	41.452	1.00	20.00
ATOM	2281	CA	LEU A 070	59.809	57.334	40.528	1.00	20.00
ATOM	2282	C	LEU A 070	59.790	58.516	39.558	1.00	20.00
ATOM	2283	O	LEU A 070	60.802	59.127	39.276	1.00	20.00
ATOM	2284	CB	LEU A 070	59.609	56.013	39.765	1.00	20.00
ATOM	2285	CG	LEU A 070	60.747	55.706	38.780	1.00	20.00
ATOM	2286	CD1	LEU A 070	61.879	55.168	39.574	1.00	20.00
ATOM	2287	CD2	LEU A 070	60.351	54.769	37.681	1.00	20.00
ATOM	2289	N	MET A 071	58.597	58.816	39.073	1.00	20.00
ATOM	2290	CA	MET A 071	58.336	59.892	38.116	1.00	20.00
ATOM	2291	C	MET A 071	59.004	61.168	38.549	1.00	20.00
ATOM	2292	O	MET A 071	59.698	61.796	37.776	1.00	20.00
ATOM	2293	CB	MET A 071	56.818	60.169	38.000	1.00	20.00

FIG. 4GG

ATOM	2294	CG	MET	A	071	56.219	59.904	36.636	1.00	20.00
ATOM	2295	SD	MET	A	071	54.409	59.761	36.764	1.00	20.00
ATOM	2296	CE	MET	A	071	53.977	58.683	35.467	1.00	20.00
ATOM	2298	N	ARG	A	072	58.797	61.527	39.803	1.00	20.00
ATOM	2299	CA	ARG	A	072	59.303	62.762	40.345	1.00	20.00
ATOM	2300	C	ARG	A	072	60.739	62.807	40.778	1.00	20.00
ATOM	2301	O	ARG	A	072	61.312	63.884	40.945	1.00	20.00
ATOM	2302	CB	ARG	A	072	58.412	63.145	41.499	1.00	20.00
ATOM	2303	CG	ARG	A	072	56.978	63.140	41.074	1.00	20.00
ATOM	2304	CD	ARG	A	072	56.500	64.539	41.064	1.00	20.00
ATOM	2305	NE	ARG	A	072	56.642	65.063	42.415	1.00	20.00
ATOM	2306	CZ	ARG	A	072	56.484	66.337	42.720	1.00	20.00
ATOM	2307	NH1	ARG	A	072	56.181	67.175	41.753	1.00	20.00
ATOM	2308	NH2	ARG	A	072	56.642	66.771	43.968	1.00	20.00
ATOM	2315	N	GLN	A	073	61.325	61.647	41.011	1.00	20.00
ATOM	2316	CA	GLN	A	073	62.717	61.652	41.387	1.00	20.00
ATOM	2317	C	GLN	A	073	63.481	61.931	40.084	1.00	20.00
ATOM	2318	O	GLN	A	073	64.658	62.267	40.105	1.00	20.00
ATOM	2319	CB	GLN	A	073	63.124	60.316	41.973	1.00	20.00
ATOM	2320	CG	GLN	A	073	63.076	60.211	43.490	1.00	20.00
ATOM	2321	CD	GLN	A	073	63.603	58.852	43.962	1.00	20.00
ATOM	2322	OE1	GLN	A	073	63.853	58.641	45.159	1.00	20.00
ATOM	2323	NE2	GLN	A	073	63.792	57.925	43.008	1.00	20.00
ATOM	2327	N	CYS	A	074	62.819	61.805	38.947	1.00	20.00
ATOM	2328	CA	CYS	A	074	63.503	62.093	37.720	1.00	20.00
ATOM	2329	C	CYS	A	074	63.403	63.601	37.500	1.00	20.00
ATOM	2330	O	CYS	A	074	64.073	64.148	36.642	1.00	20.00
ATOM	2331	CB	CYS	A	074	62.847	61.361	36.524	1.00	20.00
ATOM	2332	SG	CYS	A	074	62.746	59.548	36.564	1.00	20.00
ATOM	2334	N	TRP	A	075	62.555	64.268	38.277	1.00	20.00
ATOM	2335	CA	TRP	A	075	62.311	65.708	38.110	1.00	20.00
ATOM	2336	C	TRP	A	075	62.906	66.552	39.231	1.00	20.00
ATOM	2337	O	TRP	A	075	62.503	67.692	39.466	1.00	20.00
ATOM	2338	CB	TRP	A	075	60.797	65.977	38.037	1.00	20.00
ATOM	2339	CG	TRP	A	075	60.090	65.403	36.830	1.00	20.00
ATOM	2340	CD1	TRP	A	075	60.586	65.308	35.565	1.00	20.00
ATOM	2341	CD2	TRP	A	075	58.768	64.834	36.789	1.00	20.00
ATOM	2342	NE1	TRP	A	075	59.669	64.720	34.751	1.00	20.00
ATOM	2343	CE2	TRP	A	075	58.542	64.416	35.468	1.00	20.00
ATOM	2344	CE3	TRP	A	075	57.755	64.634	37.742	1.00	20.00
ATOM	2345	CZ2	TRP	A	075	57.343	63.808	35.062	1.00	20.00
ATOM	2346	CZ3	TRP	A	075	56.551	64.024	37.331	1.00	20.00
ATOM	2347	CH2	TRP	A	075	56.366	63.624	36.002	1.00	20.00
ATOM	2350	N	ARG	A	076	63.865	65.959	39.934	1.00	20.00
ATOM	2351	CA	ARG	A	076	64.533	66.625	41.024	1.00	20.00
ATOM	2352	C	ARG	A	076	65.304	67.793	40.364	1.00	20.00
ATOM	2353	O	ARG	A	076	65.983	67.586	39.347	1.00	20.00
ATOM	2354	CB	ARG	A	076	65.462	65.607	41.699	1.00	20.00
ATOM	2355	CG	ARG	A	076	64.890	64.932	42.981	1.00	20.00
ATOM	2356	CD	ARG	A	076	65.230	63.413	43.072	1.00	20.00
ATOM	2357	NE	ARG	A	076	64.997	62.813	44.416	1.00	20.00
ATOM	2358	CZ	ARG	A	076	65.490	61.630	44.835	1.00	20.00
ATOM	2359	NH1	ARG	A	076	66.258	60.880	44.037	1.00	20.00
ATOM	2360	NH2	ARG	A	076	65.231	61.211	46.069	1.00	20.00
ATOM	2367	N	GLU	A	077	65.178	69.014	40.895	1.00	20.00
ATOM	2368	CA	GLU	A	077	65.885	70.155	40.318	1.00	20.00
ATOM	2369	C	GLU	A	077	67.310	69.773	39.983	1.00	20.00

FIG. 4HH

ATOM	2370	O	GLU	A	077	67.613	69.364	38.878	1.00	20.00
ATOM	2371	CE	GLU	A	077	65.889	71.343	41.278	1.00	20.00
ATOM	2373	N	LYS	A	078	68.184	69.910	40.953	1.00	20.00
ATOM	2374	CA	LYS	A	078	69.573	69.583	40.764	1.00	20.00
ATOM	2375	C	LYS	A	078	69.811	68.228	40.037	1.00	20.00
ATOM	2376	O	LYS	A	078	69.850	67.194	40.664	1.00	20.00
ATOM	2377	CB	LYS	A	078	70.225	69.573	42.138	1.00	20.00
ATOM	2378	CG	LYS	A	078	69.346	70.070	43.275	1.00	20.00
ATOM	2379	CD	LYS	A	078	70.069	69.962	44.591	1.00	20.00
ATOM	2380	CE	LYS	A	078	69.301	70.580	45.713	1.00	20.00
ATOM	2381	NZ	LYS	A	078	69.362	69.789	47.005	1.00	20.00
ATOM	2386	N	PRO	A	079	70.050	68.234	38.721	1.00	20.00
ATOM	2387	CA	PRO	A	079	70.261	66.980	38.006	1.00	20.00
ATOM	2388	C	PRO	A	079	70.943	65.885	38.771	1.00	20.00
ATOM	2389	O	PRO	A	079	70.451	64.770	38.811	1.00	20.00
ATOM	2390	CB	PRO	A	079	71.059	67.370	36.772	1.00	20.00
ATOM	2391	CG	PRO	A	079	70.896	68.782	36.633	1.00	20.00
ATOM	2392	CD	PRO	A	079	70.218	69.385	37.832	1.00	20.00
ATOM	2393	N	TYR	A	080	72.085	66.172	39.382	1.00	20.00
ATOM	2394	CA	TYR	A	080	72.804	65.132	40.133	1.00	20.00
ATOM	2395	C	TYR	A	080	71.975	64.531	41.286	1.00	20.00
ATOM	2396	O	TYR	A	080	72.444	63.680	42.014	1.00	20.00
ATOM	2397	CB	TYR	A	080	74.139	65.707	40.640	1.00	20.00
ATOM	2398	CG	TYR	A	080	74.006	66.804	41.677	1.00	20.00
ATOM	2399	CD1	TYR	A	080	74.086	66.521	43.022	1.00	20.00
ATOM	2400	CD2	TYR	A	080	73.757	68.117	41.304	1.00	20.00
ATOM	2401	CE1	TYR	A	080	73.915	67.500	43.955	1.00	20.00
ATOM	2402	CE2	TYR	A	080	73.588	69.104	42.245	1.00	20.00
ATOM	2403	CZ	TYR	A	080	73.664	68.784	43.562	1.00	20.00
ATOM	2404	OH	TYR	A	080	73.475	69.749	44.512	1.00	20.00
ATOM	2407	N	GLU	A	081	70.743	65.007	41.436	1.00	20.00
ATOM	2408	CA	GLU	A	081	69.817	64.540	42.462	1.00	20.00
ATOM	2409	C	GLU	A	081	68.878	63.538	41.797	1.00	20.00
ATOM	2410	O	GLU	A	081	68.205	62.751	42.451	1.00	20.00
ATOM	2411	CB	GLU	A	081	69.025	65.709	43.038	1.00	20.00
ATOM	2412	CG	GLU	A	081	69.358	66.053	44.505	1.00	20.00
ATOM	2413	CD	GLU	A	081	68.385	67.067	45.106	1.00	20.00
ATOM	2414	OE1	GLU	A	081	68.518	67.413	46.316	1.00	20.00
ATOM	2415	OE2	GLU	A	081	67.485	67.510	44.342	1.00	20.00
ATOM	2417	N	ARG	A	082	68.875	63.582	40.471	1.00	20.00
ATOM	2418	CA	ARG	A	082	68.097	62.678	39.655	1.00	20.00
ATOM	2419	C	ARG	A	082	68.622	61.223	39.710	1.00	20.00
ATOM	2420	O	ARG	A	082	69.814	60.963	39.981	1.00	20.00
ATOM	2421	CB	ARG	A	082	68.085	63.174	38.218	1.00	20.00
ATOM	2422	CG	ARG	A	082	66.784	63.856	37.837	1.00	20.00
ATOM	2423	CD	ARG	A	082	66.836	65.398	37.781	1.00	20.00
ATOM	2424	NE	ARG	A	082	67.235	65.908	36.451	1.00	20.00
ATOM	2425	CZ	ARG	A	082	67.427	67.194	36.163	1.00	20.00
ATOM	2426	NH1	ARG	A	082	67.258	68.107	37.101	1.00	20.00
ATOM	2427	NH2	ARG	A	082	67.805	67.552	34.947	1.00	20.00
ATOM	2434	N	PRO	A	083	67.725	60.237	39.513	1.00	20.00
ATOM	2435	CA	PRO	A	083	68.223	58.866	39.554	1.00	20.00
ATOM	2436	C	PRO	A	083	69.042	58.596	38.310	1.00	20.00
ATOM	2437	O	PRO	A	083	69.594	59.505	37.688	1.00	20.00
ATOM	2438	CB	PRO	A	083	66.942	58.037	39.582	1.00	20.00
ATOM	2439	CG	PRO	A	083	65.877	58.981	40.016	1.00	20.00
ATOM	2440	CD	PRO	A	083	66.265	60.243	39.330	1.00	20.00

FIG. 4II

ATOM	2441	N	SER A 084	69.110	57.327	37.952	1.00	20.00
ATOM	2442	CA	SER A 084	69.825	56.896	36.760	1.00	20.00
ATOM	2443	C	SER A 084	69.131	55.647	36.225	1.00	20.00
ATOM	2444	O	SER A 084	68.707	54.760	36.990	1.00	20.00
ATOM	2445	CB	SER A 084	71.283	56.583	37.087	1.00	20.00
ATOM	2446	OG	SER A 084	71.397	55.714	38.182	1.00	20.00
ATOM	2449	N	PHE A 085	69.014	55.585	34.905	1.00	20.00
ATOM	2450	CA	PHE A 085	68.378	54.457	34.249	1.00	20.00
ATOM	2451	C	PHE A 085	68.808	53.087	34.761	1.00	20.00
ATOM	2452	O	PHE A 085	68.185	52.089	34.478	1.00	20.00
ATOM	2453	CB	PHE A 085	68.633	54.555	32.762	1.00	20.00
ATOM	2454	CG	PHE A 085	68.121	55.805	32.170	1.00	20.00
ATOM	2455	CD1	PHE A 085	68.888	56.546	31.303	1.00	20.00
ATOM	2456	CD2	PHE A 085	66.866	56.277	32.507	1.00	20.00
ATOM	2457	CE1	PHE A 085	68.402	57.738	30.784	1.00	20.00
ATOM	2458	CE2	PHE A 085	66.395	57.456	31.995	1.00	20.00
ATOM	2459	CZ	PHE A 085	67.160	58.174	31.140	1.00	20.00
ATOM	2461	N	ALA A 086	69.890	53.030	35.509	1.00	20.00
ATOM	2462	CA	ALA A 086	70.327	51.757	35.993	1.00	20.00
ATOM	2463	C	ALA A 086	69.505	51.422	37.206	1.00	20.00
ATOM	2464	O	ALA A 086	69.064	50.291	37.352	1.00	20.00
ATOM	2465	CB	ALA A 086	71.777	51.807	36.323	1.00	20.00
ATOM	2467	N	GLN A 087	69.266	52.398	38.071	1.00	20.00
ATOM	2468	CA	GLN A 087	68.494	52.121	39.266	1.00	20.00
ATOM	2469	C	GLN A 087	66.956	52.163	39.068	1.00	20.00
ATOM	2470	O	GLN A 087	66.195	51.560	39.846	1.00	20.00
ATOM	2471	CB	GLN A 087	68.936	53.074	40.388	1.00	20.00
ATOM	2472	CG	GLN A 087	69.565	54.391	39.973	1.00	20.00
ATOM	2473	CD	GLN A 087	70.381	55.057	41.121	1.00	20.00
ATOM	2474	OE1	GLN A 087	71.123	56.032	40.897	1.00	20.00
ATOM	2475	NE2	GLN A 087	70.244	54.536	42.341	1.00	20.00
ATOM	2479	N	ILE A 088	66.533	52.883	38.025	1.00	20.00
ATOM	2480	CA	ILE A 088	65.126	53.054	37.686	1.00	20.00
ATOM	2481	C	ILE A 088	64.687	51.697	37.241	1.00	20.00
ATOM	2482	O	ILE A 088	63.649	51.196	37.639	1.00	20.00
ATOM	2483	CB	ILE A 088	64.938	54.057	36.496	1.00	20.00
ATOM	2484	CG1	ILE A 088	64.769	55.490	37.007	1.00	20.00
ATOM	2485	CG2	ILE A 088	63.729	53.684	35.655	1.00	20.00
ATOM	2486	CD1	ILE A 088	65.373	56.556	36.035	1.00	20.00
ATOM	2488	N	LEU A 089	65.515	51.128	36.379	1.00	20.00
ATOM	2489	CA	LEU A 089	65.313	49.789	35.843	1.00	20.00
ATOM	2490	C	LEU A 089	65.060	48.826	36.994	1.00	20.00
ATOM	2491	O	LEU A 089	64.018	48.175	37.061	1.00	20.00
ATOM	2492	CB	LEU A 089	66.540	49.336	35.092	1.00	20.00
ATOM	2493	CG	LEU A 089	66.547	47.848	34.823	1.00	20.00
ATOM	2494	CD1	LEU A 089	65.147	47.379	34.407	1.00	20.00
ATOM	2495	CD2	LEU A 089	67.545	47.575	33.708	1.00	20.00
ATOM	2497	N	VAL A 090	66.004	48.748	37.908	1.00	20.00
ATOM	2498	CA	VAL A 090	65.821	47.903	39.051	1.00	20.00
ATOM	2499	C	VAL A 090	64.572	48.276	39.816	1.00	20.00
ATOM	2500	O	VAL A 090	64.276	47.684	40.843	1.00	20.00
ATOM	2501	CB	VAL A 090	66.998	48.040	39.968	1.00	20.00
ATOM	2502	CG1	VAL A 090	66.566	48.001	41.390	1.00	20.00
ATOM	2503	CG2	VAL A 090	68.012	46.942	39.655	1.00	20.00
ATOM	2505	N	SER A 091	63.807	49.232	39.295	1.00	20.00
ATOM	2506	CA	SER A 091	62.626	49.777	39.990	1.00	20.00
ATOM	2507	C	SER A 091	61.224	49.394	39.462	1.00	20.00

FIG. 4JJ

ATOM	2508	O	SER	A	091	60.265	49.286	40.228	1.00	20.00
ATOM	2509	CB	SER	A	091	62.780	51.317	40.030	1.00	20.00
ATOM	2510	OG	SER	A	091	63.064	51.756	41.334	1.00	20.00
ATOM	2513	N	LEU	A	092	61.125	49.264	38.146	1.00	20.00
ATOM	2514	CA	LEU	A	092	59.906	48.874	37.485	1.00	20.00
ATOM	2515	C	LEU	A	092	59.997	47.345	37.496	1.00	20.00
ATOM	2516	O	LEU	A	092	58.987	46.643	37.662	1.00	20.00
ATOM	2517	CB	LEU	A	092	59.941	49.394	36.065	1.00	20.00
ATOM	2518	CG	LEU	A	092	60.797	50.625	35.992	1.00	20.00
ATOM	2519	CD1	LEU	A	092	60.882	51.169	34.601	1.00	20.00
ATOM	2520	CD2	LEU	A	092	60.174	51.616	36.871	1.00	20.00
ATOM	2522	N	ASN	A	093	61.243	46.886	37.306	1.00	20.00
ATOM	2523	CA	ASN	A	093	61.699	45.495	37.299	1.00	20.00
ATOM	2524	C	ASN	A	093	61.214	44.889	38.582	1.00	20.00
ATOM	2525	O	ASN	A	093	60.803	43.724	38.635	1.00	20.00
ATOM	2526	CB	ASN	A	093	63.206	45.466	37.438	1.00	20.00
ATOM	2527	CG	ASN	A	093	63.927	44.920	36.244	1.00	20.00
ATOM	2528	OD1	ASN	A	093	65.126	44.666	36.350	1.00	20.00
ATOM	2529	ND2	ASN	A	093	63.245	44.739	35.117	1.00	20.00
ATOM	2533	N	ARG	A	094	61.344	45.693	39.631	1.00	20.00
ATOM	2534	CA	ARG	A	094	60.992	45.309	40.985	1.00	20.00
ATOM	2535	C	ARG	A	094	59.515	45.614	41.318	1.00	20.00
ATOM	2536	O	ARG	A	094	59.112	45.717	42.468	1.00	20.00
ATOM	2537	CB	ARG	A	094	61.954	46.010	41.937	1.00	20.00
ATOM	2538	CG	ARG	A	094	61.850	45.571	43.339	1.00	20.00
ATOM	2539	CD	ARG	A	094	62.088	46.747	44.262	1.00	20.00
ATOM	2540	NE	ARG	A	094	61.170	46.917	45.403	1.00	20.00
ATOM	2541	CZ	ARG	A	094	59.842	47.007	45.328	1.00	20.00
ATOM	2542	NH1	ARG	A	094	59.224	46.948	44.164	1.00	20.00
ATOM	2543	NH2	ARG	A	094	59.129	47.209	46.438	1.00	20.00
ATOM	2550	N	MET	A	095	58.710	45.750	40.278	1.00	20.00
ATOM	2551	CA	MET	A	095	57.306	46.018	40.421	1.00	20.00
ATOM	2552	C	MET	A	095	56.723	44.944	39.527	1.00	20.00
ATOM	2553	O	MET	A	095	55.597	44.512	39.706	1.00	20.00
ATOM	2554	CB	MET	A	095	56.967	47.406	39.870	1.00	20.00
ATOM	2555	CG	MET	A	095	57.240	48.556	40.822	1.00	20.00
ATOM	2556	SD	MET	A	095	56.618	50.279	40.365	1.00	20.00
ATOM	2557	CE	MET	A	095	56.509	50.955	42.056	1.00	20.00
ATOM	2559	N	LEU	A	096	57.495	44.509	38.551	1.00	20.00
ATOM	2560	CA	LEU	A	096	57.034	43.476	37.646	1.00	20.00
ATOM	2561	C	LEU	A	096	56.931	42.034	38.341	1.00	20.00
ATOM	2562	O	LEU	A	096	56.594	40.999	37.738	1.00	20.00
ATOM	2563	CB	LEU	A	096	57.960	43.493	36.401	1.00	20.00
ATOM	2564	CG	LEU	A	096	57.892	44.684	35.421	1.00	20.00
ATOM	2565	CD1	LEU	A	096	58.856	44.515	34.311	1.00	20.00
ATOM	2566	CD2	LEU	A	096	56.523	44.804	34.819	1.00	20.00
ATOM	2568	N	GLU	A	097	57.181	41.981	39.633	1.00	20.00
ATOM	2569	CA	GLU	A	097	57.102	40.734	40.327	1.00	20.00
ATOM	2570	C	GLU	A	097	56.396	40.934	41.642	1.00	20.00
ATOM	2571	O	GLU	A	097	57.064	41.042	42.664	1.00	20.00
ATOM	2572	CB	GLU	A	097	58.499	40.252	40.606	1.00	20.00
ATOM	2573	CG	GLU	A	097	59.459	40.519	39.475	1.00	20.00
ATOM	2574	CD	GLU	A	097	60.327	39.305	39.212	1.00	20.00
ATOM	2575	OE1	GLU	A	097	60.756	38.703	40.228	1.00	20.00
ATOM	2576	OE2	GLU	A	097	60.564	38.961	38.022	1.00	20.00
ATOM	2578	N	GLU	A	098	55.062	41.010	41.622	1.00	20.00
ATOM	2579	CA	GLU	A	098	54.192	41.177	42.823	1.00	20.00

ATOM	2580	C	GLU	A	098	52.812	41.404	42.219	1.00	20.00
ATOM	2581	O	GLU	A	098	51.765	41.462	42.905	1.00	20.00
ATOM	2582	CB	GLU	A	098	54.514	42.433	43.686	1.00	20.00
ATOM	2583	CG	GLU	A	098	55.726	43.286	43.421	1.00	20.00
ATOM	2584	CD	GLU	A	098	56.655	43.318	44.654	1.00	20.00
ATOM	2585	OE1	GLU	A	098	56.157	43.414	45.803	1.00	20.00
ATOM	2586	OE2	GLU	A	098	57.903	43.232	44.488	1.00	20.00
ATOM	2588	N	ARG	A	099	52.872	41.529	40.898	1.00	20.00
ATOM	2589	CA	ARG	A	099	51.725	41.820	40.069	1.00	20.00
ATOM	2590	C	ARG	A	099	50.664	42.484	40.859	1.00	20.00
ATOM	2591	O	ARG	A	099	49.536	41.992	40.902	1.00	20.00
ATOM	2592	CB	ARG	A	099	51.107	40.600	39.385	1.00	20.00
ATOM	2593	CG	ARG	A	099	50.252	41.009	38.173	1.00	20.00
ATOM	2594	CD	ARG	A	099	49.462	42.327	38.402	1.00	20.00
ATOM	2595	NE	ARG	A	099	48.780	42.813	37.193	1.00	20.00
ATOM	2596	CZ	ARG	A	099	48.995	44.001	36.614	1.00	20.00
ATOM	2597	NH1	ARG	A	099	49.888	44.858	37.132	1.00	20.00
ATOM	2598	NH2	ARG	A	099	48.348	44.319	35.492	1.00	20.00
ATOM	2605	N	LYS	A	100	51.012	43.593	41.491	1.00	20.00
ATOM	2606	CA	LYS	A	100	49.996	44.273	42.208	1.00	20.00
ATOM	2607	C	LYS	A	100	49.233	45.314	41.412	1.00	20.00
ATOM	2608	O	LYS	A	100	48.414	46.009	41.961	1.00	20.00
ATOM	2609	CB	LYS	A	100	50.568	44.887	43.452	1.00	20.00
ATOM	2610	CG	LYS	A	100	49.723	44.455	44.606	1.00	20.00
ATOM	2611	CD	LYS	A	100	48.746	43.295	44.135	1.00	20.00
ATOM	2612	CE	LYS	A	100	47.476	43.250	44.951	1.00	20.00
ATOM	2613	NZ	LYS	A	100	47.799	42.986	46.386	1.00	20.00
ATOM	2618	N	THR	A	101	49.448	45.372	40.107	1.00	20.00
ATOM	2619	CA	THR	A	101	48.825	46.402	39.284	1.00	20.00
ATOM	2620	C	THR	A	101	49.208	47.748	39.873	1.00	20.00
ATOM	2621	O	THR	A	101	48.788	48.131	40.984	1.00	20.00
ATOM	2622	CB	THR	A	101	47.325	46.313	39.223	1.00	20.00
ATOM	2623	OG1	THR	A	101	46.859	45.424	40.224	1.00	20.00
ATOM	2624	CG2	THR	A	101	46.913	45.840	37.852	1.00	20.00
ATOM	2627	N	TYR	A	102	50.025	48.453	39.098	1.00	20.00
ATOM	2628	CA	TYR	A	102	50.547	49.712	39.515	1.00	20.00
ATOM	2629	C	TYR	A	102	49.870	50.826	38.785	1.00	20.00
ATOM	2630	O	TYR	A	102	49.661	51.891	39.342	1.00	20.00
ATOM	2631	CB	TYR	A	102	52.040	49.684	39.310	1.00	20.00
ATOM	2632	CG	TYR	A	102	52.744	48.940	40.406	1.00	20.00
ATOM	2633	CD1	TYR	A	102	53.416	47.744	40.169	1.00	20.00
ATOM	2634	CD2	TYR	A	102	52.769	49.460	41.663	1.00	20.00
ATOM	2635	CE1	TYR	A	102	54.090	47.122	41.160	1.00	20.00
ATOM	2636	CE2	TYR	A	102	53.430	48.852	42.653	1.00	20.00
ATOM	2637	CZ	TYR	A	102	54.102	47.691	42.416	1.00	20.00
ATOM	2638	OH	TYR	A	102	54.846	47.188	43.470	1.00	20.00
ATOM	2641	N	VAL	A	103	49.568	50.591	37.524	1.00	20.00
ATOM	2642	CA	VAL	A	103	48.790	51.544	36.741	1.00	20.00
ATOM	2643	C	VAL	A	103	47.512	50.735	36.788	1.00	20.00
ATOM	2644	O	VAL	A	103	47.571	49.547	37.137	1.00	20.00
ATOM	2645	CB	VAL	A	103	49.121	51.597	35.265	1.00	20.00
ATOM	2646	CG1	VAL	A	103	48.387	52.783	34.645	1.00	20.00
ATOM	2647	CG2	VAL	A	103	50.633	51.634	35.049	1.00	20.00
ATOM	2649	N	ASN	A	104	46.380	51.336	36.420	1.00	20.00
ATOM	2650	CA	ASN	A	104	45.109	50.645	36.473	1.00	20.00
ATOM	2651	C	ASN	A	104	44.386	51.023	35.231	1.00	20.00
ATOM	2652	O	ASN	A	104	44.569	52.110	34.731	1.00	20.00

FIG. 4LL

ATOM	2653	CB	ASN	A	104	44.360	51.089	37.714	1.00	20.00
ATOM	2654	CG	ASN	A	104	42.863	51.071	37.544	1.00	20.00
ATOM	2655	OD1	ASN	A	104	42.348	51.013	36.431	1.00	20.00
ATOM	2656	ND2	ASN	A	104	42.149	51.139	38.666	1.00	20.00
ATOM	2660	N	THR	A	105	43.545	50.137	34.732	1.00	20.00
ATOM	2661	CA	THR	A	105	42.855	50.390	33.490	1.00	20.00
ATOM	2662	C	THR	A	105	41.412	49.870	33.596	1.00	20.00
ATOM	2663	O	THR	A	105	40.678	49.783	32.593	1.00	20.00
ATOM	2664	CB	THR	A	105	43.627	49.686	32.341	1.00	20.00
ATOM	2665	OG1	THR	A	105	44.293	48.501	32.839	1.00	20.00
ATOM	2666	CG2	THR	A	105	44.686	50.595	31.792	1.00	20.00
ATOM	2669	N	THR	A	106	41.013	49.565	34.831	1.00	20.00
ATOM	2670	CA	THR	A	106	39.701	49.048	35.173	1.00	20.00
ATOM	2671	C	THR	A	106	38.588	50.103	35.353	1.00	20.00
ATOM	2672	O	THR	A	106	38.818	51.077	36.038	1.00	20.00
ATOM	2673	CB	THR	A	106	39.850	48.258	36.473	1.00	20.00
ATOM	2674	OG1	THR	A	106	39.615	46.869	36.226	1.00	20.00
ATOM	2675	CG2	THR	A	106	38.902	48.779	37.552	1.00	20.00
ATOM	2678	N	LEU	A	107	37.383	49.891	34.775	1.00	20.00
ATOM	2679	CA	LEU	A	107	36.229	50.816	34.903	1.00	20.00
ATOM	2680	C	LEU	A	107	35.437	50.546	36.199	1.00	20.00
ATOM	2681	O	LEU	A	107	35.067	49.413	36.473	1.00	20.00
ATOM	2682	CB	LEU	A	107	35.279	50.655	33.739	1.00	20.00
ATOM	2683	CG	LEU	A	107	35.798	50.744	32.313	1.00	20.00
ATOM	2684	CD1	LEU	A	107	34.625	50.728	31.345	1.00	20.00
ATOM	2685	CD2	LEU	A	107	36.667	51.987	32.120	1.00	20.00
ATOM	2687	N	TYR	A	108	35.176	51.583	36.998	1.00	20.00
ATOM	2688	CA	TYR	A	108	34.436	51.444	38.260	1.00	20.00
ATOM	2689	C	TYR	A	108	33.529	52.660	38.590	1.00	20.00
ATOM	2690	O	TYR	A	108	33.124	52.843	39.767	1.00	20.00
ATOM	2691	CB	TYR	A	108	35.417	51.219	39.419	1.00	20.00
ATOM	2692	CG	TYR	A	108	36.234	49.960	39.165	1.00	20.00
ATOM	2693	CD1	TYR	A	108	37.446	49.725	40.176	1.00	20.00
ATOM	2694	CD2	TYR	A	108	35.201	48.850	39.201	1.00	20.00
ATOM	2696	N	GLU	A	109	33.228	53.475	37.565	1.00	20.00
ATOM	2697	CA	GLU	A	109	32.363	54.664	37.691	1.00	20.00
ATOM	2698	C	GLU	A	109	33.115	55.935	37.364	1.00	20.00
ATOM	2699	O	GLU	A	109	34.039	56.360	38.093	1.00	20.00
ATOM	2700	CB	GLU	A	109	31.764	54.786	39.092	1.00	20.00
ATOM	2702	N	LYS	A	110	32.723	56.590	36.284	1.00	20.00
ATOM	2703	CA	LYS	A	110	33.431	57.801	35.968	1.00	20.00
ATOM	2704	C	LYS	A	110	34.879	57.443	35.586	1.00	20.00
ATOM	2705	O	LYS	A	110	35.653	56.902	36.366	1.00	20.00
ATOM	2706	CB	LYS	A	110	33.373	58.742	37.176	1.00	20.00
ATOM	2707	CG	LYS	A	110	32.211	58.399	38.165	1.00	20.00
ATOM	2708	CD	LYS	A	110	31.414	59.597	38.754	1.00	20.00
ATOM	2709	CE	LYS	A	110	30.154	59.092	39.514	1.00	20.00
ATOM	2710	NZ	LYS	A	110	30.320	58.678	40.967	1.00	20.00
ATOM	2715	N	PHE	A	111	35.184	57.675	34.324	1.00	20.00
ATOM	2716	CA	PHE	A	111	36.489	57.460	33.833	1.00	20.00
ATOM	2717	C	PHE	A	111	36.665	58.179	32.520	1.00	20.00
ATOM	2718	O	PHE	A	111	36.065	57.840	31.494	1.00	20.00
ATOM	2719	CB	PHE	A	111	36.842	55.994	33.658	1.00	20.00
ATOM	2720	CG	PHE	A	111	38.193	55.795	33.013	1.00	20.00
ATOM	2721	CD1	PHE	A	111	39.337	55.675	33.772	1.00	20.00
ATOM	2722	CD2	PHE	A	111	38.332	55.861	31.657	1.00	20.00
ATOM	2723	CE1	PHE	A	111	40.601	55.639	33.171	1.00	20.00

FIG. 4MM

ATOM	2724	CE2	PHE	A	111	39.575	55.824	31.077	1.00	20.00
ATOM	2725	CZ	PHE	A	111	40.706	55.717	31.830	1.00	20.00
ATOM	2727	N	THR	A	112	37.540	59.180	32.584	1.00	20.00
ATOM	2728	CA	THR	A	112	37.904	59.997	31.457	1.00	20.00
ATOM	2729	C	THR	A	112	39.374	59.703	31.350	1.00	20.00
ATOM	2730	O	THR	A	112	39.967	59.297	32.329	1.00	20.00
ATOM	2731	CB	THR	A	112	37.686	61.487	31.794	1.00	20.00
ATOM	2732	OG1	THR	A	112	36.780	61.598	32.899	1.00	20.00
ATOM	2733	CG2	THR	A	112	37.079	62.216	30.623	1.00	20.00
ATOM	2736	N	TYR	A	113	39.926	59.880	30.153	1.00	20.00
ATOM	2737	CA	TYR	A	113	41.339	59.706	29.866	1.00	20.00
ATOM	2738	C	TYR	A	113	42.092	61.000	30.123	1.00	20.00
ATOM	2739	O	TYR	A	113	41.837	61.669	31.105	1.00	20.00
ATOM	2740	CB	TYR	A	113	41.520	59.320	28.433	1.00	20.00
ATOM	2741	CG	TYR	A	113	41.095	57.923	28.236	1.00	20.00
ATOM	2742	CD1	TYR	A	113	40.063	57.606	27.346	1.00	20.00
ATOM	2743	CD2	TYR	A	113	41.699	56.879	28.960	1.00	20.00
ATOM	2744	CE1	TYR	A	113	39.641	56.300	27.178	1.00	20.00
ATOM	2745	CE2	TYR	A	113	41.283	55.573	28.792	1.00	20.00
ATOM	2746	CZ	TYR	A	113	40.251	55.291	27.894	1.00	20.00
ATOM	2747	OH	TYR	A	113	39.853	53.992	27.670	1.00	20.00
ATOM	2750	N	ALA	A	114	42.958	61.423	29.201	1.00	20.00
ATOM	2751	CA	ALA	A	114	43.754	62.605	29.511	1.00	20.00
ATOM	2752	C	ALA	A	114	43.947	63.838	28.571	1.00	20.00
ATOM	2753	O	ALA	A	114	43.604	64.944	28.952	1.00	20.00
ATOM	2754	CB	ALA	A	114	45.129	62.109	30.025	1.00	20.00
ATOM	2756	N	GLY	A	115	44.491	63.670	27.377	1.00	20.00
ATOM	2757	CA	GLY	A	115	44.727	64.815	26.532	1.00	20.00
ATOM	2758	C	GLY	A	115	44.350	64.834	25.059	1.00	20.00
ATOM	2759	O	GLY	A	115	45.029	64.291	24.173	1.00	20.00
ATOM	2761	N	ILE	A	116	43.220	65.504	24.838	1.00	20.00
ATOM	2762	CA	ILE	A	116	42.609	65.779	23.527	1.00	20.00
ATOM	2763	C	ILE	A	116	41.516	64.772	23.037	1.00	20.00
ATOM	2764	O	ILE	A	116	41.123	63.952	23.880	1.00	20.00
ATOM	2765	CB	ILE	A	116	43.744	65.993	22.469	1.00	20.00
ATOM	2766	OXT	ILE	A	116	41.049	64.815	21.867	1.00	20.00
TER										
HETATM	1	C1	INH3A		1	58.776	51.045	11.645	0.00	0.00
HETATM	2	N2	INH3A		1	58.172	52.218	11.841	0.00	0.00
HETATM	3	C3	INH3A		1	58.936	53.310	12.056	0.00	0.00
HETATM	4	C4	INH3A		1	60.320	53.244	12.077	0.00	0.00
HETATM	5	C5	INH3A		1	60.887	51.924	11.859	0.00	0.00
HETATM	6	N6	INH3A		1	60.101	50.854	11.646	0.00	0.00
HETATM	8	N8	INH3A		1	58.497	54.604	12.288	0.00	0.00
HETATM	9	C9	INH3A		1	59.673	55.293	12.446	0.00	0.00
HETATM	10	C10	INH3A		1	60.842	54.525	12.326	0.00	0.00
HETATM	12	N13	INH3A		1	62.289	51.734	11.876	0.00	0.00
HETATM	13	C14	INH3A		1	62.258	54.972	12.430	0.00	0.00
HETATM	14	C16	INH3A		1	57.098	55.079	12.339	0.00	0.00
HETATM	15	C17	INH3A		1	63.049	54.530	13.477	0.00	0.00
HETATM	16	C18	INH3A		1	64.374	54.941	13.612	0.00	0.00
HETATM	17	C19	INH3A		1	64.935	55.815	12.687	0.00	0.00
HETATM	18	C20	INH3A		1	64.131	56.249	11.643	0.00	0.00
HETATM	19	C21	INH3A		1	62.810	55.841	11.508	0.00	0.00
HETATM	23	N25	INH3A		1	66.225	56.236	12.788	0.00	0.00
HETATM	24	S26	INH3A		1	66.995	56.113	14.217	0.00	0.00
HETATM	25	O27	INH3A		1	65.999	55.773	15.187	0.00	0.00

FIG. 4NN

HETATM	26	O28	INH3A	1	67.770	57.301	14.420	0.00	0.00
HETATM	27	C29	INH3A	1	68.100	54.741	14.032	0.00	0.00
HETATM	28	C30	INH3A	1	69.041	54.751	13.007	0.00	0.00
HETATM	29	C31	INH3A	1	69.873	53.654	12.825	0.00	0.00
HETATM	30	C32	INH3A	1	69.740	52.566	13.674	0.00	0.00
HETATM	31	C33	INH3A	1	68.801	52.539	14.696	0.00	0.00
HETATM	32	C34	INH3A	1	67.972	53.639	14.872	0.00	0.00
HETATM	37	F39	INH3A	1	70.540	51.507	13.502	0.00	0.00
HETATM	39	F41	INH3A	1	64.638	57.094	10.735	0.00	0.00
HETATM	40	C42	INH3A	1	56.781	55.784	13.669	0.00	0.00
HETATM	41	C43	INH3A	1	55.311	56.219	13.720	0.00	0.00
HETATM	42	C44	INH3A	1	54.962	57.130	12.528	0.00	0.00
HETATM	43	C45	INH3A	1	55.278	56.419	11.202	0.00	0.00
HETATM	44	C46	INH3A	1	56.748	55.981	11.144	0.00	0.00
HETATM	53	C55	INH3A	1	53.385	58.715	13.548	0.00	0.00
HETATM	54	C56	INH3A	1	51.998	59.356	13.419	0.00	0.00
HETATM	55	N57	INH3A	1	50.930	58.353	13.520	0.00	0.00
HETATM	56	C58	INH3A	1	51.136	57.302	12.516	0.00	0.00
HETATM	57	C59	INH3A	1	52.522	56.662	12.658	0.00	0.00
HETATM	58	N60	INH3A	1	53.588	57.668	12.536	0.00	0.00
HETATM	68	C70	INH3A	1	49.599	58.958	13.416	0.00	0.00
TER									

FIG. 400

CRYST	86.000	86.000	112.000	90.00	90.00	90.00	P42212
SCALE1	0.01163	0.00000	0.00000			0.00000	
SCALE2	0.00000	0.01163	0.00000			0.00000	
SCALE3	0.00000	0.00000	0.00893			0.00000	
ATOM	1	N	PRO A 817	8.606	38.803	6.968	1.00 63.06
ATOM	2	CA	PRO A 817	9.750	39.629	6.436	1.00 62.53
ATOM	3	C	PRO A 817	10.180	38.953	5.133	1.00 62.97
ATOM	4	O	PRO A 817	10.749	37.851	5.149	1.00 59.85
ATOM	5	CB	PRO A 817	10.807	39.752	7.499	1.00 62.45
ATOM	6	N	VAL A 818	9.794	39.542	3.998	1.00 63.22
ATOM	7	CA	VAL A 818	10.112	38.916	2.711	1.00 66.18
ATOM	8	C	VAL A 818	11.172	39.708	1.952	1.00 67.24
ATOM	9	O	VAL A 818	11.086	40.927	1.837	1.00 68.73
ATOM	10	CB	VAL A 818	8.866	38.691	1.843	1.00 66.96
ATOM	11	CG1	VAL A 818	9.133	37.632	0.770	1.00 67.29
ATOM	12	CG2	VAL A 818	7.637	38.224	2.629	1.00 66.80
ATOM	13	N	LEU A 819	12.192	39.014	1.464	1.00 67.40
ATOM	14	CA	LEU A 819	13.300	39.569	0.705	1.00 67.89
ATOM	15	C	LEU A 819	13.445	38.938	-0.680	1.00 68.53
ATOM	16	O	LEU A 819	13.179	37.750	-0.875	1.00 67.98
ATOM	17	CB	LEU A 819	14.589	39.374	1.493	1.00 67.17
ATOM	18	N	ASP A 820	13.854	39.728	-1.668	1.00 70.32
ATOM	19	CA	ASP A 820	13.962	39.181	-3.018	1.00 74.15
ATOM	20	C	ASP A 820	15.382	38.826	-3.421	1.00 75.07
ATOM	21	O	ASP A 820	16.390	39.377	-2.978	1.00 74.87
ATOM	22	CB	ASP A 820	13.314	40.147	-4.017	1.00 76.15
ATOM	23	CG	ASP A 820	13.968	41.518	-4.054	1.00 78.23
ATOM	24	OD1	ASP A 820	14.712	41.846	-3.092	1.00 79.04
ATOM	25	OD2	ASP A 820	13.712	42.246	-5.051	1.00 78.55
ATOM	26	N	TRP A 821	15.489	37.870	-4.336	1.00 77.12
ATOM	27	CA	TRP A 821	16.794	37.480	-4.871	1.00 80.00
ATOM	28	C	TRP A 821	17.288	38.671	-5.674	1.00 80.90
ATOM	29	O	TRP A 821	16.560	39.677	-5.750	1.00 82.56
ATOM	30	CB	TRP A 821	16.640	36.237	-5.738	1.00 81.50
ATOM	31	CG	TRP A 821	17.979	35.683	-6.126	1.00 84.29
ATOM	32	CD1	TRP A 821	18.770	36.052	-7.174	1.00 85.04
ATOM	33	CD2	TRP A 821	18.686	34.639	-5.443	1.00 85.54
ATOM	34	NE1	TRP A 821	19.932	35.323	-7.184	1.00 85.91
ATOM	35	CE2	TRP A 821	19.895	34.435	-6.138	1.00 86.16
ATOM	36	CE3	TRP A 821	18.402	33.854	-4.317	1.00 85.72
ATOM	37	CZ2	TRP A 821	20.822	33.474	-5.736	1.00 86.76
ATOM	38	CZ3	TRP A 821	19.317	32.899	-3.914	1.00 86.12
ATOM	39	CH2	TRP A 821	20.513	32.723	-4.632	1.00 86.81
ATOM	40	N	ASN A 822	18.490	38.703	-6.220	1.00 80.99
ATOM	41	CA	ASN A 822	18.941	39.868	-6.995	1.00 81.52
ATOM	42	C	ASN A 822	18.729	41.071	-6.079	1.00 80.56
ATOM	43	O	ASN A 822	18.110	42.084	-6.381	1.00 81.67
ATOM	44	CB	ASN A 822	18.164	39.937	-8.312	1.00 83.00
ATOM	45	CG	ASN A 822	19.059	40.084	-9.532	1.00 84.08
ATOM	46	OD1	ASN A 822	20.168	40.617	-9.420	1.00 84.25
ATOM	47	ND2	ASN A 822	18.581	39.608	-10.679	1.00 84.49
ATOM	48	N	ASP A 823	19.204	40.923	-4.856	1.00 78.69
ATOM	49	CA	ASP A 823	19.120	41.815	-3.723	1.00 76.89
ATOM	50	C	ASP A 823	19.874	41.123	-2.568	1.00 74.92
ATOM	51	O	ASP A 823	19.952	41.542	-1.417	1.00 75.11
ATOM	52	CB	ASP A 823	17.695	42.112	-3.299	1.00 77.66
ATOM	53	CG	ASP A 823	17.306	43.572	-3.217	1.00 78.83

FIG. 5A

ATOM	54	OD1	ASP	A	823	17.885	44.406	-3.955	1.00	79.53
ATOM	55	OD2	ASP	A	823	16.391	43.945	-2.444	1.00	78.52
ATOM	56	N	ILE	A	824	20.438	39.973	-2.919	1.00	71.67
ATOM	57	CA	ILE	A	824	21.270	39.189	-2.030	1.00	69.30
ATOM	58	C	ILE	A	824	22.624	39.046	-2.750	1.00	67.35
ATOM	59	O	ILE	A	824	22.678	38.352	-3.770	1.00	65.47
ATOM	60	CB	ILE	A	824	20.744	37.783	-1.696	1.00	69.43
ATOM	61	CG1	ILE	A	824	19.356	37.733	-1.074	1.00	69.93
ATOM	62	CG2	ILE	A	824	21.752	37.046	-0.820	1.00	69.07
ATOM	63	CD1	ILE	A	824	19.156	38.009	0.386	1.00	71.48
ATOM	64	N	LYS	A	825	23.649	39.735	-2.252	1.00	65.03
ATOM	65	CA	LYS	A	825	24.977	39.581	-2.829	1.00	63.66
ATOM	66	C	LYS	A	825	25.810	38.677	-1.903	1.00	62.88
ATOM	67	O	LYS	A	825	26.290	39.103	-0.850	1.00	60.46
ATOM	68	CB	LYS	A	825	25.688	40.893	-3.082	1.00	63.33
ATOM	69	N	PHE	A	826	25.952	37.420	-2.315	1.00	62.22
ATOM	70	CA	PHE	A	826	26.745	36.434	-1.595	1.00	63.65
ATOM	71	C	PHE	A	826	28.243	36.752	-1.654	1.00	64.85
ATOM	72	O	PHE	A	826	28.806	36.978	-2.738	1.00	65.98
ATOM	73	CB	PHE	A	826	26.535	35.019	-2.151	1.00	63.23
ATOM	74	CG	PHE	A	826	25.242	34.324	-1.828	1.00	63.28
ATOM	75	CD1	PHE	A	826	24.194	34.262	-2.742	1.00	63.47
ATOM	76	CD2	PHE	A	826	25.068	33.738	-0.587	1.00	62.78
ATOM	77	CE1	PHE	A	826	23.013	33.606	-2.421	1.00	63.26
ATOM	78	CE2	PHE	A	826	23.893	33.090	-0.261	1.00	63.76
ATOM	79	CZ	PHE	A	826	22.859	33.026	-1.183	1.00	63.42
ATOM	80	N	GLN	A	827	28.933	36.771	-0.514	1.00	64.73
ATOM	81	CA	GLN	A	827	30.359	37.048	-0.474	1.00	63.67
ATOM	82	C	GLN	A	827	31.182	35.763	-0.387	1.00	62.27
ATOM	83	O	GLN	A	827	31.703	35.217	-1.356	1.00	61.84
ATOM	84	CB	GLN	A	827	30.736	37.884	0.748	1.00	65.45
ATOM	85	CG	GLN	A	827	29.641	38.676	1.428	1.00	69.14
ATOM	86	CD	GLN	A	827	29.805	40.166	1.185	1.00	71.09
ATOM	87	OE1	GLN	A	827	29.364	40.617	0.124	1.00	72.36
ATOM	88	NE2	GLN	A	827	30.442	40.865	2.124	1.00	71.89
ATOM	89	N	ASP	A	828	31.371	35.286	0.838	1.00	61.57
ATOM	90	CA	ASP	A	828	32.237	34.122	1.034	1.00	62.37
ATOM	91	C	ASP	A	828	31.576	33.071	1.883	1.00	61.37
ATOM	92	O	ASP	A	828	30.330	32.899	1.910	1.00	63.34
ATOM	93	CB	ASP	A	828	33.605	34.623	1.532	1.00	63.30
ATOM	94	CG	ASP	A	828	33.536	35.073	2.977	1.00	65.22
ATOM	95	OD1	ASP	A	828	34.629	35.346	3.505	1.00	66.32
ATOM	96	OD2	ASP	A	828	32.418	35.135	3.513	1.00	67.27
ATOM	97	N	VAL	A	829	32.332	32.174	2.503	1.00	59.16
ATOM	98	CA	VAL	A	829	31.820	31.095	3.339	1.00	56.81
ATOM	99	C	VAL	A	829	32.101	31.413	4.805	1.00	57.13
ATOM	100	O	VAL	A	829	33.252	31.767	5.119	1.00	57.41
ATOM	101	CB	VAL	A	829	32.462	29.753	2.948	1.00	55.58
ATOM	102	CG1	VAL	A	829	32.035	28.658	3.909	1.00	55.56
ATOM	103	CG2	VAL	A	829	32.111	29.383	1.513	1.00	55.17
ATOM	104	N	ILE	A	830	31.106	31.314	5.693	1.00	56.36
ATOM	105	CA	ILE	A	830	31.360	31.613	7.108	1.00	54.69
ATOM	106	C	ILE	A	830	31.971	30.371	7.750	1.00	54.51
ATOM	107	O	ILE	A	830	32.927	30.411	8.507	1.00	54.88
ATOM	108	CB	ILE	A	830	30.170	32.157	7.898	1.00	52.84
ATOM	109	CG1	ILE	A	830	29.780	33.560	7.374	1.00	52.48
ATOM	110	CG2	ILE	A	830	30.518	32.300	9.375	1.00	51.14

FIG. 5B

ATOM	111	CD1	ILE	A	830	28.389	34.012	7.808	1.00	52.01
ATOM	112	N	GLY	A	831	31.431	29.232	7.376	1.00	54.93
ATOM	113	CA	GLY	A	831	31.949	27.959	7.866	1.00	57.73
ATOM	114	C	GLY	A	831	30.703	27.066	7.878	1.00	60.30
ATOM	115	O	GLY	A	831	29.687	27.433	7.281	1.00	59.66
ATOM	116	N	GLU	A	832	30.811	25.963	8.594	1.00	62.36
ATOM	117	CA	GLU	A	832	29.649	25.080	8.634	1.00	65.54
ATOM	118	C	GLU	A	832	28.918	25.256	9.956	1.00	67.03
ATOM	119	O	GLU	A	832	29.525	25.480	10.982	1.00	65.58
ATOM	120	CB	GLU	A	832	30.079	23.647	8.389	1.00	65.24
ATOM	121	CG	GLU	A	832	29.979	22.748	9.615	1.00	64.68
ATOM	122	CD	GLU	A	832	30.771	21.493	9.247	1.00	65.38
ATOM	123	OE1	GLU	A	832	31.871	21.394	9.838	1.00	65.15
ATOM	124	OE2	GLU	A	832	30.232	20.771	8.386	1.00	64.01
ATOM	125	N	GLY	A	833	27.605	25.128	9.870	1.00	71.16
ATOM	126	CA	GLY	A	833	26.741	25.268	11.048	1.00	75.85
ATOM	127	C	GLY	A	833	25.973	23.945	11.138	1.00	79.10
ATOM	128	O	GLY	A	833	26.489	22.959	11.666	1.00	80.05
ATOM	129	N	ASN	A	834	24.750	23.982	10.627	1.00	80.77
ATOM	130	CA	ASN	A	834	23.887	22.807	10.614	1.00	82.57
ATOM	131	C	ASN	A	834	23.055	22.917	9.332	1.00	82.72
ATOM	132	O	ASN	A	834	22.709	24.047	8.973	1.00	83.47
ATOM	133	CB	ASN	A	834	22.974	22.712	11.826	1.00	83.64
ATOM	134	CG	ASN	A	834	23.565	22.227	13.122	1.00	84.87
ATOM	135	OD1	ASN	A	834	23.040	22.476	14.214	1.00	85.57
ATOM	136	ND2	ASN	A	834	24.692	21.516	13.114	1.00	85.28
ATOM	137	N	PHE	A	835	22.813	21.799	8.663	1.00	82.37
ATOM	138	CA	PHE	A	835	22.018	21.747	7.436	1.00	81.44
ATOM	139	C	PHE	A	835	22.770	22.311	6.227	1.00	79.71
ATOM	140	O	PHE	A	835	22.207	22.742	5.221	1.00	80.02
ATOM	141	CB	PHE	A	835	20.656	22.423	7.609	1.00	81.62
ATOM	142	N	GLY	A	836	24.093	22.257	6.306	1.00	77.25
ATOM	143	CA	GLY	A	836	25.011	22.771	5.308	1.00	73.64
ATOM	144	C	GLY	A	836	25.714	24.008	5.875	1.00	70.61
ATOM	145	O	GLY	A	836	25.485	24.453	7.008	1.00	71.32
ATOM	146	N	GLN	A	837	26.589	24.607	5.081	1.00	67.00
ATOM	147	CA	GLN	A	837	27.288	25.779	5.584	1.00	64.94
ATOM	148	C	GLN	A	837	26.303	26.943	5.749	1.00	61.14
ATOM	149	O	GLN	A	837	25.079	26.947	5.627	1.00	62.09
ATOM	150	CB	GLN	A	837	28.510	26.214	4.782	1.00	65.56
ATOM	151	CG	GLN	A	837	28.323	26.175	3.277	1.00	68.22
ATOM	152	CD	GLN	A	837	28.499	24.771	2.717	1.00	70.10
ATOM	153	OE1	GLN	A	837	27.540	23.989	2.498	1.00	71.35
ATOM	154	NE2	GLN	A	837	29.776	24.447	2.508	1.00	69.74
ATOM	155	N	VAL	A	838	26.949	27.991	6.223	1.00	56.19
ATOM	156	CA	VAL	A	838	26.368	29.284	6.530	1.00	52.12
ATOM	157	C	VAL	A	838	27.166	30.196	5.612	1.00	51.49
ATOM	158	O	VAL	A	838	28.401	30.088	5.669	1.00	50.02
ATOM	159	CB	VAL	A	838	26.657	29.586	8.002	1.00	50.54
ATOM	160	CG1	VAL	A	838	26.258	30.989	8.386	1.00	48.67
ATOM	161	CG2	VAL	A	838	25.974	28.553	8.890	1.00	48.75
ATOM	162	N	LEU	A	839	26.512	30.915	4.719	1.00	50.28
ATOM	163	CA	LEU	A	839	27.308	31.782	3.831	1.00	48.12
ATOM	164	C	LEU	A	839	27.210	33.217	4.324	1.00	48.21
ATOM	165	O	LEU	A	839	26.364	33.580	5.139	1.00	46.74
ATOM	166	CB	LEU	A	839	26.831	31.625	2.395	1.00	47.75
ATOM	167	CG	LEU	A	839	26.828	30.229	1.803	1.00	48.45

FIG. 5C

ATOM	168	CD1	LEU	A	839	26.155	30.260	0.433	1.00	47.96
ATOM	169	CD2	LEU	A	839	28.160	29.519	1.717	1.00	44.56
ATOM	170	N	LYS	A	840	28.053	34.107	3.847	1.00	47.52
ATOM	171	CA	LYS	A	840	27.984	35.508	4.234	1.00	48.47
ATOM	172	C	LYS	A	840	27.434	36.369	3.109	1.00	49.26
ATOM	173	O	LYS	A	840	27.837	36.150	1.960	1.00	49.21
ATOM	174	CB	LYS	A	840	29.393	35.943	4.654	1.00	48.66
ATOM	175	CG	LYS	A	840	29.320	37.059	5.668	1.00	49.85
ATOM	176	CD	LYS	A	840	29.716	38.398	5.125	1.00	49.60
ATOM	177	CE	LYS	A	840	29.768	39.457	6.225	1.00	50.13
ATOM	178	NZ	LYS	A	840	31.184	39.749	6.580	1.00	51.35
ATOM	179	N	ALA	A	841	26.486	37.270	3.389	1.00	51.52
ATOM	180	CA	ALA	A	841	25.968	38.108	2.312	1.00	53.29
ATOM	181	C	ALA	A	841	25.768	39.564	2.726	1.00	54.51
ATOM	182	O	ALA	A	841	25.753	39.914	3.903	1.00	54.20
ATOM	183	CB	ALA	A	841	24.641	37.503	1.837	1.00	52.47
ATOM	184	N	ARG	A	842	25.564	40.398	1.714	1.00	57.16
ATOM	185	CA	ARG	A	842	25.154	41.784	1.915	1.00	60.23
ATOM	186	C	ARG	A	842	23.699	41.667	1.451	1.00	61.88
ATOM	187	O	ARG	A	842	23.499	41.023	0.416	1.00	63.40
ATOM	188	CB	ARG	A	842	25.900	42.835	1.119	1.00	61.09
ATOM	189	CG	ARG	A	842	27.301	43.137	1.622	1.00	62.77
ATOM	190	CD	ARG	A	842	27.258	43.791	2.995	1.00	63.72
ATOM	191	NE	ARG	A	842	26.985	45.231	2.928	1.00	64.65
ATOM	192	CZ	ARG	A	842	26.963	45.986	4.017	1.00	65.52
ATOM	193	NH1	ARG	A	842	26.724	47.291	4.022	1.00	65.78
ATOM	194	NH2	ARG	A	842	27.158	45.436	5.214	1.00	66.80
ATOM	195	N	ILE	A	843	22.745	42.047	2.281	1.00	63.86
ATOM	196	CA	ILE	A	843	21.322	41.935	1.983	1.00	66.38
ATOM	197	C	ILE	A	843	20.610	43.284	2.150	1.00	69.29
ATOM	198	O	ILE	A	843	20.337	43.810	3.233	1.00	72.01
ATOM	199	CB	ILE	A	843	20.524	40.846	2.715	1.00	64.76
ATOM	200	CG1	ILE	A	843	20.218	41.134	4.182	1.00	63.75
ATOM	201	CG2	ILE	A	843	21.198	39.477	2.638	1.00	65.06
ATOM	202	CD1	ILE	A	843	19.030	40.372	4.733	1.00	61.60
ATOM	203	N	LYS	A	844	20.274	43.844	0.975	1.00	70.72
ATOM	204	CA	LYS	A	844	19.599	45.144	0.939	1.00	72.14
ATOM	205	C	LYS	A	844	18.157	45.087	1.427	1.00	73.85
ATOM	206	O	LYS	A	844	17.234	44.834	0.650	1.00	74.26
ATOM	207	CB	LYS	A	844	19.596	45.771	-0.449	1.00	71.35
ATOM	208	N	LYS	A	845	17.931	45.392	2.697	1.00	75.42
ATOM	209	CA	LYS	A	845	16.580	45.403	3.262	1.00	77.81
ATOM	210	C	LYS	A	845	16.190	46.868	3.403	1.00	80.30
ATOM	211	O	LYS	A	845	16.751	47.630	4.197	1.00	79.71
ATOM	212	CB	LYS	A	845	16.528	44.624	4.561	1.00	77.32
ATOM	213	CG	LYS	A	845	15.188	44.450	5.231	1.00	76.89
ATOM	214	CD	LYS	A	845	15.318	43.734	6.572	1.00	76.27
ATOM	215	CE	LYS	A	845	13.956	43.469	7.205	1.00	75.52
ATOM	216	NZ	LYS	A	845	14.066	42.788	8.521	1.00	74.44
ATOM	217	N	ASP	A	846	15.243	47.333	2.610	1.00	82.92
ATOM	218	CA	ASP	A	846	14.674	48.627	2.374	1.00	84.85
ATOM	219	C	ASP	A	846	15.649	49.493	1.560	1.00	85.22
ATOM	220	O	ASP	A	846	15.804	49.302	0.353	1.00	85.44
ATOM	221	CB	ASP	A	846	14.070	49.395	3.514	1.00	86.44
ATOM	222	CG	ASP	A	846	14.770	49.744	4.790	1.00	87.92
ATOM	223	OD1	ASP	A	846	15.058	50.942	5.029	1.00	88.52
ATOM	224	OD2	ASP	A	846	15.044	48.819	5.599	1.00	89.21

FIG. 5D

ATOM	225	N	GLY	A	847	16.337	50.395	2.231	1.00	85.08
ATOM	226	CA	GLY	A	847	17.317	51.266	1.590	1.00	83.96
ATOM	227	C	GLY	A	847	18.593	51.154	2.430	1.00	83.43
ATOM	228	O	GLY	A	847	19.555	51.871	2.210	1.00	84.91
ATOM	229	N	LEU	A	848	18.493	50.239	3.396	1.00	81.24
ATOM	230	CA	LEU	A	848	19.634	49.951	4.250	1.00	78.49
ATOM	231	C	LEU	A	848	20.311	48.732	3.617	1.00	76.61
ATOM	232	O	LEU	A	848	19.608	47.760	3.340	1.00	76.98
ATOM	233	CB	LEU	A	848	19.195	49.564	5.658	1.00	78.88
ATOM	234	CG	LEU	A	848	18.312	50.582	6.388	1.00	79.08
ATOM	235	CD1	LEU	A	848	17.346	49.858	7.312	1.00	79.29
ATOM	236	CD2	LEU	A	848	19.184	51.563	7.157	1.00	79.32
ATOM	237	N	ARG	A	849	21.592	48.863	3.326	1.00	73.72
ATOM	238	CA	ARG	A	849	22.332	47.696	2.850	1.00	70.15
ATOM	239	C	ARG	A	849	22.830	47.095	4.175	1.00	67.06
ATOM	240	O	ARG	A	849	23.153	47.922	5.036	1.00	65.85
ATOM	241	CB	ARG	A	849	23.493	48.031	1.941	1.00	71.56
ATOM	242	CG	ARG	A	849	23.308	47.798	0.452	1.00	72.96
ATOM	243	CD	ARG	A	849	24.483	46.995	-0.110	1.00	74.22
ATOM	244	NE	ARG	A	849	25.606	47.792	-0.586	1.00	75.64
ATOM	245	CZ	ARG	A	849	26.848	47.399	-0.871	1.00	75.22
ATOM	246	NH1	ARG	A	849	27.183	46.121	-0.715	1.00	73.54
ATOM	247	NH2	ARG	A	849	27.739	48.290	-1.305	1.00	74.94
ATOM	248	N	MET	A	850	22.777	45.781	4.369	1.00	63.25
ATOM	249	CA	MET	A	850	23.293	45.285	5.655	1.00	59.28
ATOM	250	C	MET	A	850	23.898	43.883	5.493	1.00	55.95
ATOM	251	O	MET	A	850	23.690	43.197	4.494	1.00	56.07
ATOM	252	CB	MET	A	850	22.245	45.279	6.757	1.00	58.62
ATOM	253	CG	MET	A	850	21.296	44.096	6.631	1.00	59.21
ATOM	254	SD	MET	A	850	19.724	44.280	7.443	1.00	59.73
ATOM	255	CE	MET	A	850	20.128	44.922	9.049	1.00	59.43
ATOM	256	N	ASP	A	851	24.651	43.563	6.548	1.00	51.79
ATOM	257	CA	ASP	A	851	25.299	42.268	6.600	1.00	48.61
ATOM	258	C	ASP	A	851	24.332	41.192	7.084	1.00	45.57
ATOM	259	O	ASP	A	851	23.630	41.457	8.086	1.00	42.14
ATOM	260	CB	ASP	A	851	26.379	42.285	7.697	1.00	50.01
ATOM	261	CG	ASP	A	851	27.669	42.933	7.256	1.00	50.84
ATOM	262	OD1	ASP	A	851	28.043	42.801	6.057	1.00	51.87
ATOM	263	OD2	ASP	A	851	28.272	43.563	8.144	1.00	50.81
ATOM	264	N	ALA	A	852	24.472	39.961	6.632	1.00	45.45
ATOM	265	CA	ALA	A	852	23.622	38.884	7.138	1.00	42.89
ATOM	266	C	ALA	A	852	24.373	37.570	7.066	1.00	42.71
ATOM	267	O	ALA	A	852	25.336	37.518	6.303	1.00	43.78
ATOM	268	CB	ALA	A	852	22.397	38.727	6.261	1.00	41.61
ATOM	269	N	ALA	A	853	23.847	36.577	7.785	1.00	43.18
ATOM	270	CA	ALA	A	853	24.394	35.222	7.668	1.00	43.19
ATOM	271	C	ALA	A	853	23.300	34.446	6.931	1.00	45.23
ATOM	272	O	ALA	A	853	22.122	34.570	7.296	1.00	45.40
ATOM	273	CB	ALA	A	853	24.725	34.651	9.043	1.00	43.45
ATOM	274	N	ILE	A	854	23.599	33.717	5.863	1.00	45.69
ATOM	275	CA	ILE	A	854	22.561	33.051	5.093	1.00	46.79
ATOM	276	C	ILE	A	854	22.583	31.537	5.228	1.00	50.11
ATOM	277	O	ILE	A	854	23.643	30.913	5.101	1.00	51.97
ATOM	278	CB	ILE	A	854	22.686	33.334	3.581	1.00	45.28
ATOM	279	CG1	ILE	A	854	22.754	34.819	3.268	1.00	45.20
ATOM	280	CG2	ILE	A	854	21.553	32.685	2.794	1.00	45.13
ATOM	281	CD1	ILE	A	854	21.509	35.654	3.433	1.00	45.48

FIG. 5E

ATOM	282	N	LYS	A	855	21.408	30.949	5.453	1.00	51.72
ATOM	283	CA	LYS	A	855	21.355	29.474	5.425	1.00	54.33
ATOM	284	C	LYS	A	855	20.240	29.052	4.458	1.00	55.89
ATOM	285	O	LYS	A	855	19.276	29.786	4.205	1.00	52.41
ATOM	286	CB	LYS	A	855	21.271	28.892	6.808	1.00	55.64
ATOM	287	CG	LYS	A	855	19.914	28.834	7.487	1.00	58.25
ATOM	288	CD	LYS	A	855	20.052	28.092	8.807	1.00	59.55
ATOM	289	CE	LYS	A	855	18.987	27.027	9.025	1.00	60.12
ATOM	290	NZ	LYS	A	855	19.484	26.165	10.151	1.00	60.89
ATOM	291	N	ARG	A	856	20.386	27.871	3.871	1.00	59.82
ATOM	292	CA	ARG	A	856	19.419	27.341	2.915	1.00	63.71
ATOM	293	C	ARG	A	856	18.809	26.009	3.309	1.00	66.24
ATOM	294	O	ARG	A	856	19.456	25.004	3.565	1.00	66.29
ATOM	295	CB	ARG	A	856	20.126	27.258	1.555	1.00	63.38
ATOM	296	N	MET	A	857	17.486	25.951	3.418	1.00	69.77
ATOM	297	CA	MET	A	857	16.718	24.748	3.728	1.00	73.04
ATOM	298	C	MET	A	857	15.960	24.381	2.447	1.00	75.83
ATOM	299	O	MET	A	857	16.149	25.126	1.472	1.00	77.44
ATOM	300	CB	MET	A	857	15.761	24.965	4.887	1.00	72.49
ATOM	301	N	LYS	A	858	15.174	23.321	2.404	1.00	78.15
ATOM	302	CA	LYS	A	858	14.449	22.985	1.184	1.00	80.35
ATOM	303	C	LYS	A	858	13.181	22.168	1.417	1.00	81.76
ATOM	304	O	LYS	A	858	13.118	21.298	2.282	1.00	82.29
ATOM	305	CB	LYS	A	858	15.320	22.196	0.212	1.00	80.34
ATOM	306	N	GLU	A	859	12.171	22.427	0.593	1.00	82.86
ATOM	307	CA	GLU	A	859	10.905	21.705	0.631	1.00	83.98
ATOM	308	C	GLU	A	859	10.372	21.378	2.024	1.00	84.84
ATOM	309	O	GLU	A	859	9.465	20.540	2.160	1.00	85.54
ATOM	310	CB	GLU	A	859	11.040	20.388	-0.143	1.00	83.34
TER										
ATOM	311	N	ASP	B	868	3.887	24.257	9.102	1.00	74.33
ATOM	312	CA	ASP	B	868	4.969	23.506	9.742	1.00	73.45
ATOM	313	C	ASP	B	868	6.151	24.465	9.894	1.00	72.92
ATOM	314	O	ASP	B	868	6.215	25.236	10.848	1.00	72.75
ATOM	315	CB	ASP	B	868	5.345	22.276	8.927	1.00	73.09
ATOM	316	N	PHE	B	869	6.973	24.491	8.845	1.00	71.93
ATOM	317	CA	PHE	B	869	8.128	25.356	8.739	1.00	71.39
ATOM	318	C	PHE	B	869	7.722	26.812	8.514	1.00	69.85
ATOM	319	O	PHE	B	869	8.507	27.721	8.789	1.00	68.53
ATOM	320	CB	PHE	B	869	9.086	24.894	7.635	1.00	72.16
ATOM	321	N	ALA	B	870	6.485	27.041	8.084	1.00	68.66
ATOM	322	CA	ALA	B	870	6.008	28.412	7.917	1.00	67.79
ATOM	323	C	ALA	B	870	5.699	28.972	9.300	1.00	66.69
ATOM	324	O	ALA	B	870	5.914	30.142	9.612	1.00	67.76
ATOM	325	CB	ALA	B	870	4.786	28.421	7.009	1.00	67.73
ATOM	326	N	GLY	B	871	5.125	28.124	10.156	1.00	64.74
ATOM	327	CA	GLY	B	871	4.746	28.539	11.506	1.00	63.48
ATOM	328	C	GLY	B	871	5.968	28.696	12.407	1.00	63.38
ATOM	329	O	GLY	B	871	6.078	29.586	13.241	1.00	62.27
ATOM	330	N	GLU	B	872	6.936	27.789	12.259	1.00	63.08
ATOM	331	CA	GLU	B	872	8.163	27.830	13.033	1.00	62.41
ATOM	332	C	GLU	B	872	8.870	29.166	12.865	1.00	59.48
ATOM	333	O	GLU	B	872	9.299	29.759	13.849	1.00	59.18
ATOM	334	CB	GLU	B	872	9.104	26.684	12.627	1.00	64.92
ATOM	335	CG	GLU	B	872	8.756	25.334	13.218	1.00	67.28
ATOM	336	CD	GLU	B	872	9.191	24.093	12.474	1.00	68.33
ATOM	337	OE1	GLU	B	872	8.848	22.953	12.910	1.00	69.51

FIG. 5F

ATOM	338	OE2	GLU	B	872	9.882	24.117	11.435	1.00	69.53
ATOM	339	N	LEU	B	873	9.004	29.664	11.648	1.00	57.71
ATOM	340	CA	LEU	B	873	9.635	30.916	11.312	1.00	55.15
ATOM	341	C	LEU	B	873	8.988	32.099	12.034	1.00	55.46
ATOM	342	O	LEU	B	873	9.656	33.045	12.483	1.00	53.19
ATOM	343	CB	LEU	B	873	9.629	31.206	9.816	1.00	54.80
ATOM	344	CG	LEU	B	873	10.436	30.326	8.876	1.00	56.52
ATOM	345	CD1	LEU	B	873	10.416	30.920	7.466	1.00	56.98
ATOM	346	CD2	LEU	B	873	11.886	30.139	9.305	1.00	57.06
ATOM	347	N	GLU	B	874	7.663	32.055	12.083	1.00	53.38
ATOM	348	CA	GLU	B	874	6.839	33.058	12.743	1.00	53.73
ATOM	349	C	GLU	B	874	7.208	33.198	14.215	1.00	50.89
ATOM	350	O	GLU	B	874	7.431	34.279	14.773	1.00	48.19
ATOM	351	CB	GLU	B	874	5.379	32.579	12.639	1.00	57.54
ATOM	352	CG	GLU	B	874	4.388	33.300	13.533	1.00	61.33
ATOM	353	CD	GLU	B	874	3.007	32.638	13.433	1.00	64.62
ATOM	354	OE1	GLU	B	874	2.075	33.216	14.045	1.00	66.21
ATOM	355	OE2	GLU	B	874	2.876	31.577	12.771	1.00	64.60
ATOM	356	N	VAL	B	875	7.278	32.004	14.839	1.00	48.16
ATOM	357	CA	VAL	B	875	7.665	31.965	16.266	1.00	47.64
ATOM	358	C	VAL	B	875	9.051	32.599	16.426	1.00	46.85
ATOM	359	O	VAL	B	875	9.211	33.498	17.257	1.00	45.14
ATOM	360	CB	VAL	B	875	7.523	30.545	16.799	1.00	47.78
ATOM	361	CG1	VAL	B	875	8.477	30.264	17.946	1.00	48.21
ATOM	362	CG2	VAL	B	875	6.077	30.272	17.240	1.00	47.41
ATOM	363	N	LEU	B	876	10.000	32.278	15.538	1.00	47.87
ATOM	364	CA	LEU	B	876	11.348	32.838	15.552	1.00	50.02
ATOM	365	C	LEU	B	876	11.435	34.322	15.245	1.00	50.20
ATOM	366	O	LEU	B	876	12.285	34.988	15.845	1.00	51.04
ATOM	367	CB	LEU	B	876	12.308	32.074	14.611	1.00	48.16
ATOM	368	CG	LEU	B	876	12.598	30.663	15.159	1.00	49.64
ATOM	369	CD1	LEU	B	876	13.303	29.816	14.116	1.00	48.69
ATOM	370	CD2	LEU	B	876	13.407	30.766	16.452	1.00	51.42
ATOM	371	N	CYS	B	877	10.607	34.849	14.358	1.00	50.72
ATOM	372	CA	CYS	B	877	10.638	36.276	14.029	1.00	51.41
ATOM	373	C	CYS	B	877	10.130	37.090	15.215	1.00	50.29
ATOM	374	O	CYS	B	877	10.630	38.171	15.550	1.00	49.69
ATOM	375	CB	CYS	B	877	9.777	36.555	12.788	1.00	53.49
ATOM	376	SG	CYS	B	877	9.320	38.304	12.668	1.00	56.75
ATOM	377	N	LYS	B	878	9.155	36.480	15.922	1.00	49.77
ATOM	378	CA	LYS	B	878	8.602	37.082	17.122	1.00	49.11
ATOM	379	C	LYS	B	878	9.567	37.033	18.298	1.00	47.30
ATOM	380	O	LYS	B	878	9.418	37.925	19.128	1.00	47.68
ATOM	381	CB	LYS	B	878	7.284	36.415	17.561	1.00	51.27
ATOM	382	CG	LYS	B	878	6.097	36.821	16.728	1.00	53.14
ATOM	383	CD	LYS	B	878	5.072	35.740	16.473	1.00	55.56
ATOM	384	CE	LYS	B	878	4.132	35.453	17.638	1.00	55.88
ATOM	385	NZ	LYS	B	878	3.445	34.138	17.433	1.00	57.41
ATOM	386	N	LEU	B	879	10.495	36.091	18.403	1.00	44.23
ATOM	387	CA	LEU	B	879	11.388	36.049	19.550	1.00	42.64
ATOM	388	C	LEU	B	879	12.665	36.881	19.317	1.00	41.06
ATOM	389	O	LEU	B	879	13.291	37.300	20.264	1.00	39.35
ATOM	390	CB	LEU	B	879	11.857	34.606	19.819	1.00	41.39
ATOM	391	CG	LEU	B	879	10.790	33.580	20.246	1.00	40.34
ATOM	392	CD1	LEU	B	879	11.327	32.180	20.076	1.00	40.43
ATOM	393	CD2	LEU	B	879	10.378	33.826	21.693	1.00	40.68
ATOM	394	N	GLY	B	880	12.974	37.194	18.075	1.00	40.80

FIG. 5G

ATOM	395	CA	GLY	B	880	14.164	37.870	17.686	1.00	42.66
ATOM	396	C	GLY	B	880	14.499	39.226	18.185	1.00	43.75
ATOM	397	O	GLY	B	880	15.698	39.526	18.103	1.00	46.29
ATOM	398	N	HIS	B	881	13.580	40.053	18.637	1.00	42.86
ATOM	399	CA	HIS	B	881	13.759	41.403	19.105	1.00	43.65
ATOM	400	C	HIS	B	881	14.619	41.378	20.370	1.00	39.48
ATOM	401	O	HIS	B	881	15.539	42.203	20.446	1.00	43.05
ATOM	402	CB	HIS	B	881	12.417	42.127	19.236	1.00	47.39
ATOM	403	CG	HIS	B	881	11.628	42.051	20.490	1.00	50.98
ATOM	404	ND1	HIS	B	881	10.412	41.442	20.685	1.00	53.62
ATOM	405	CD2	HIS	B	881	11.944	42.576	21.711	1.00	53.62
ATOM	406	CE1	HIS	B	881	10.057	41.591	21.975	1.00	55.27
ATOM	407	NE2	HIS	B	881	10.966	42.286	22.647	1.00	55.05
ATOM	408	N	HIS	B	882	14.422	40.401	21.250	1.00	35.00
ATOM	409	CA	HIS	B	882	15.234	40.280	22.473	1.00	33.75
ATOM	410	C	HIS	B	882	16.695	40.394	22.053	1.00	29.63
ATOM	411	O	HIS	B	882	17.099	39.702	21.115	1.00	32.51
ATOM	412	CB	HIS	B	882	14.977	38.947	23.240	1.00	29.31
ATOM	413	CG	HIS	B	882	15.458	39.007	24.665	1.00	28.91
ATOM	414	ND1	HIS	B	882	16.739	38.861	25.208	1.00	28.25
ATOM	415	CD2	HIS	B	882	14.687	39.334	25.705	1.00	27.99
ATOM	416	CE1	HIS	B	882	16.623	39.049	26.523	1.00	28.98
ATOM	417	NE2	HIS	B	882	15.346	39.333	26.866	1.00	26.63
ATOM	418	N	PRO	B	883	17.468	41.252	22.659	1.00	31.32
ATOM	419	CA	PRO	B	883	18.882	41.398	22.375	1.00	31.40
ATOM	420	C	PRO	B	883	19.687	40.158	22.658	1.00	32.62
ATOM	421	O	PRO	B	883	20.700	39.965	21.941	1.00	36.70
ATOM	422	CB	PRO	B	883	19.206	42.672	23.123	1.00	30.55
ATOM	423	CG	PRO	B	883	18.433	42.543	24.437	1.00	33.27
ATOM	424	CD	PRO	B	883	17.096	42.064	23.858	1.00	31.21
ATOM	425	N	ASN	B	884	19.290	39.189	23.448	1.00	33.73
ATOM	426	CA	ASN	B	884	19.999	37.942	23.685	1.00	32.47
ATOM	427	C	ASN	B	884	19.496	36.811	22.823	1.00	34.37
ATOM	428	O	ASN	B	884	19.901	35.659	23.051	1.00	34.65
ATOM	429	CB	ASN	B	884	19.952	37.596	25.173	1.00	33.46
ATOM	430	CG	ASN	B	884	20.404	38.649	26.117	1.00	36.23
ATOM	431	OD1	ASN	B	884	20.011	39.181	27.122	1.00	37.73
ATOM	432	ND2	ASN	B	884	21.749	38.992	25.840	1.00	32.70
ATOM	433	N	ILE	B	885	18.623	37.014	21.825	1.00	32.48
ATOM	434	CA	ILE	B	885	18.185	36.032	20.859	1.00	34.12
ATOM	435	C	ILE	B	885	18.587	36.426	19.455	1.00	32.76
ATOM	436	O	ILE	B	885	18.359	37.539	18.982	1.00	33.37
ATOM	437	CB	ILE	B	885	16.662	35.743	21.004	1.00	33.83
ATOM	438	CG1	ILE	B	885	16.442	35.119	22.402	1.00	35.22
ATOM	439	CG2	ILE	B	885	16.088	34.847	19.922	1.00	33.58
ATOM	440	CD1	ILE	B	885	14.970	34.840	22.653	1.00	38.35
ATOM	441	N	ILE	B	886	19.261	35.557	18.697	1.00	34.99
ATOM	442	CA	ILE	B	886	19.694	35.965	17.333	1.00	37.58
ATOM	443	C	ILE	B	886	18.478	36.272	16.468	1.00	39.01
ATOM	444	O	ILE	B	886	17.526	35.459	16.453	1.00	38.20
ATOM	445	CB	ILE	B	886	20.693	34.967	16.752	1.00	38.15
ATOM	446	CG1	ILE	B	886	21.549	35.590	15.622	1.00	40.28
ATOM	447	CG2	ILE	B	886	19.985	33.776	16.206	1.00	38.96
ATOM	448	CD1	ILE	B	886	22.675	36.445	16.190	1.00	39.25
ATOM	449	N	ASN	B	887	18.472	37.380	15.731	1.00	38.67
ATOM	450	CA	ASN	B	887	17.268	37.824	15.016	1.00	40.23
ATOM	451	C	ASN	B	887	17.116	37.485	13.560	1.00	40.18

FIG. 5H

ATOM	452	O	ASN	B	887	18.061	37.480	12.780	1.00	41.35
ATOM	453	CB	ASN	B	887	17.153	39.347	15.231	1.00	40.41
ATOM	454	CG	ASN	B	887	15.888	39.999	14.697	1.00	40.25
ATOM	455	OD1	ASN	B	887	15.961	41.166	14.290	1.00	39.53
ATOM	456	ND2	ASN	B	887	14.746	39.340	14.692	1.00	38.70
ATOM	457	N	LEU	B	888	15.891	37.146	13.147	1.00	42.05
ATOM	458	CA	LEU	B	888	15.624	36.781	11.744	1.00	43.89
ATOM	459	C	LEU	B	888	15.501	38.053	10.900	1.00	44.52
ATOM	460	O	LEU	B	888	14.790	38.957	11.351	1.00	42.69
ATOM	461	CB	LEU	B	888	14.321	35.988	11.680	1.00	45.35
ATOM	462	CG	LEU	B	888	13.675	35.835	10.310	1.00	46.44
ATOM	463	CD1	LEU	B	888	14.617	35.185	9.322	1.00	47.08
ATOM	464	CD2	LEU	B	888	12.393	35.011	10.433	1.00	48.74
ATOM	465	N	LEU	B	889	16.221	38.160	9.785	1.00	46.33
ATOM	466	CA	LEU	B	889	16.106	39.377	9.004	1.00	48.96
ATOM	467	C	LEU	B	889	15.178	39.162	7.822	1.00	48.91
ATOM	468	O	LEU	B	889	14.331	40.055	7.642	1.00	52.61
ATOM	469	CB	LEU	B	889	17.407	40.091	8.621	1.00	52.03
ATOM	470	CG	LEU	B	889	18.022	40.806	9.850	1.00	54.44
ATOM	471	CD1	LEU	B	889	18.709	39.713	10.624	1.00	56.62
ATOM	472	CD2	LEU	B	889	19.053	41.862	9.535	1.00	56.92
ATOM	473	N	GLY	B	890	15.192	38.056	7.122	1.00	48.86
ATOM	474	CA	GLY	B	890	14.281	37.806	6.027	1.00	49.19
ATOM	475	C	GLY	B	890	14.348	36.393	5.478	1.00	51.62
ATOM	476	O	GLY	B	890	15.216	35.581	5.811	1.00	49.54
ATOM	477	N	ALA	B	891	13.367	36.080	4.619	1.00	52.67
ATOM	478	CA	ALA	B	891	13.339	34.779	3.956	1.00	55.84
ATOM	479	C	ALA	B	891	13.195	35.036	2.454	1.00	58.68
ATOM	480	O	ALA	B	891	12.782	36.128	2.056	1.00	60.04
ATOM	481	CB	ALA	B	891	12.292	33.826	4.471	1.00	54.13
ATOM	482	N	CYS	B	892	13.681	34.109	1.646	1.00	61.71
ATOM	483	CA	CYS	B	892	13.618	34.248	0.200	1.00	64.65
ATOM	484	C	CYS	B	892	13.505	32.847	-0.403	1.00	67.70
ATOM	485	O	CYS	B	892	14.279	31.955	-0.046	1.00	68.56
ATOM	486	CB	CYS	B	892	14.817	34.942	-0.412	1.00	63.99
ATOM	487	SG	CYS	B	892	14.859	34.973	-2.216	1.00	64.16
ATOM	488	N	GLU	B	893	12.506	32.682	-1.262	1.00	70.26
ATOM	489	CA	GLU	B	893	12.337	31.411	-1.965	1.00	72.47
ATOM	490	C	GLU	B	893	12.959	31.542	-3.354	1.00	72.44
ATOM	491	O	GLU	B	893	12.603	32.421	-4.134	1.00	72.20
ATOM	492	CB	GLU	B	893	10.873	30.991	-2.027	1.00	74.16
ATOM	493	CG	GLU	B	893	10.291	30.437	-0.736	1.00	76.17
ATOM	494	CD	GLU	B	893	8.789	30.210	-0.801	1.00	77.74
ATOM	495	OE1	GLU	B	893	8.126	30.906	-1.611	1.00	78.37
ATOM	496	OE2	GLU	B	893	8.230	29.357	-0.069	1.00	78.86
ATOM	497	N	HIS	B	894	13.922	30.697	-3.677	1.00	73.54
ATOM	498	CA	HIS	B	894	14.594	30.700	-4.977	1.00	74.67
ATOM	499	C	HIS	B	894	14.847	29.255	-5.401	1.00	74.91
ATOM	500	O	HIS	B	894	15.025	28.386	-4.542	1.00	74.35
ATOM	501	CB	HIS	B	894	15.857	31.531	-4.919	1.00	75.48
ATOM	502	CG	HIS	B	894	16.558	31.697	-6.225	1.00	76.90
ATOM	503	ND1	HIS	B	894	17.369	30.719	-6.752	1.00	77.63
ATOM	504	CD2	HIS	B	894	16.587	32.733	-7.097	1.00	77.64
ATOM	505	CE1	HIS	B	894	17.880	31.150	-7.893	1.00	78.14
ATOM	506	NE2	HIS	B	894	17.433	32.377	-8.119	1.00	77.87
ATOM	507	N	ARG	B	895	14.774	28.959	-6.699	1.00	74.84
ATOM	508	CA	ARG	B	895	14.865	27.593	-7.214	1.00	73.98

FIG. 5I.

ATOM	509	C	ARG	B	895	14.001	26.742	-6.281	1.00	74.16
ATOM	510	O	ARG	B	895	12.911	27.249	-5.967	1.00	74.67
ATOM	511	CB	ARG	B	895	16.262	27.053	-7.367	1.00	74.14
ATOM	512	N	GLY	B	896	14.429	25.597	-5.769	1.00	73.62
ATOM	513	CA	GLY	B	896	13.554	24.843	-4.878	1.00	74.58
ATOM	514	C	GLY	B	896	13.801	24.946	-3.383	1.00	75.31
ATOM	515	O	GLY	B	896	13.362	24.085	-2.599	1.00	74.62
ATOM	516	N	TYR	B	897	14.568	25.958	-2.952	1.00	75.55
ATOM	517	CA	TYR	B	897	14.937	26.107	-1.551	1.00	75.78
ATOM	518	C	TYR	B	897	14.498	27.408	-0.882	1.00	73.41
ATOM	519	O	TYR	B	897	14.296	28.420	-1.548	1.00	73.50
ATOM	520	CB	TYR	B	897	16.466	26.038	-1.444	1.00	78.25
ATOM	521	CG	TYR	B	897	17.225	24.811	-1.836	1.00	80.53
ATOM	522	CD1	TYR	B	897	17.259	24.356	-3.145	1.00	81.37
ATOM	523	CD2	TYR	B	897	17.982	24.114	-0.898	1.00	81.11
ATOM	524	CE1	TYR	B	897	17.983	23.232	-3.498	1.00	82.95
ATOM	525	CE2	TYR	B	897	18.712	22.994	-1.247	1.00	82.00
ATOM	526	CZ	TYR	B	897	18.723	22.542	-2.554	1.00	82.42
ATOM	527	N	LEU	B	898	14.434	27.417	0.450	1.00	70.37
ATOM	528	CA	LEU	B	898	14.132	28.667	1.172	1.00	68.25
ATOM	529	C	LEU	B	898	15.407	29.218	1.794	1.00	66.94
ATOM	530	O	LEU	B	898	16.271	28.530	2.340	1.00	67.22
ATOM	531	CB	LEU	B	898	12.957	28.443	2.089	1.00	67.63
ATOM	532	CG	LEU	B	898	12.979	28.839	3.549	1.00	66.92
ATOM	533	CD1	LEU	B	898	11.612	29.212	4.063	1.00	67.30
ATOM	534	CD2	LEU	B	898	13.492	27.667	4.393	1.00	67.72
ATOM	535	N	TYR	B	899	15.648	30.512	1.585	1.00	65.23
ATOM	536	CA	TYR	B	899	16.871	31.191	2.019	1.00	61.95
ATOM	537	C	TYR	B	899	16.601	32.001	3.262	1.00	60.81
ATOM	538	O	TYR	B	899	15.646	32.797	3.247	1.00	61.40
ATOM	539	CB	TYR	B	899	17.291	31.923	0.733	1.00	62.33
ATOM	540	CG	TYR	B	899	17.999	31.028	-0.267	1.00	63.29
ATOM	541	CD1	TYR	B	899	17.347	30.060	-1.018	1.00	63.92
ATOM	542	CD2	TYR	B	899	19.373	31.154	-0.439	1.00	63.86
ATOM	543	CE1	TYR	B	899	18.025	29.235	-1.897	1.00	64.75
ATOM	544	CE2	TYR	B	899	20.078	30.345	-1.317	1.00	64.65
ATOM	545	CZ	TYR	B	899	19.395	29.384	-2.041	1.00	65.94
ATOM	546	OH	TYR	B	899	20.089	28.577	-2.918	1.00	66.41
ATOM	547	N	LEU	B	900	17.269	31.750	4.397	1.00	56.58
ATOM	548	CA	LEU	B	900	17.006	32.506	5.625	1.00	52.46
ATOM	549	C	LEU	B	900	18.209	33.421	5.892	1.00	50.69
ATOM	550	O	LEU	B	900	19.359	33.002	5.834	1.00	49.63
ATOM	551	CB	LEU	B	900	16.742	31.664	6.859	1.00	52.94
ATOM	552	CG	LEU	B	900	15.786	30.472	6.845	1.00	53.46
ATOM	553	CD1	LEU	B	900	16.449	29.204	6.312	1.00	53.02
ATOM	554	CD2	LEU	B	900	15.211	30.153	8.224	1.00	53.76
ATOM	555	N	ALA	B	901	17.923	34.696	6.093	1.00	48.07
ATOM	556	CA	ALA	B	901	18.972	35.699	6.337	1.00	44.87
ATOM	557	C	ALA	B	901	18.893	36.119	7.800	1.00	42.43
ATOM	558	O	ALA	B	901	17.895	36.689	8.253	1.00	41.24
ATOM	559	CB	ALA	B	901	18.777	36.899	5.429	1.00	43.13
ATOM	560	N	ILE	B	902	19.919	35.717	8.532	1.00	42.59
ATOM	561	CA	ILE	B	902	20.012	35.929	9.979	1.00	40.02
ATOM	562	C	ILE	B	902	20.926	37.088	10.334	1.00	40.16
ATOM	563	O	ILE	B	902	21.844	37.413	9.586	1.00	41.22
ATOM	564	CB	ILE	B	902	20.561	34.648	10.635	1.00	39.22
ATOM	565	CG1	ILE	B	902	19.781	33.405	10.190	1.00	41.67

ATOM	566	CG2	ILE	B	902	20.538	34.742	12.152	1.00	38.02
ATOM	567	CD1	ILE	B	902	18.288	33.542	10.392	1.00	44.70
ATOM	568	N	GLU	B	903	20.702	37.692	11.498	1.00	38.24
ATOM	569	CA	GLU	B	903	21.487	38.756	12.058	1.00	36.51
ATOM	570	C	GLU	B	903	22.929	38.231	12.121	1.00	37.45
ATOM	571	O	GLU	B	903	23.188	37.096	12.569	1.00	37.05
ATOM	572	CB	GLU	B	903	20.984	39.024	13.484	1.00	36.53
ATOM	573	CG	GLU	B	903	21.936	39.865	14.343	1.00	39.44
ATOM	574	CD	GLU	B	903	21.384	40.070	15.735	1.00	40.57
ATOM	575	OE1	GLU	B	903	21.848	40.909	16.534	1.00	39.27
ATOM	576	OE2	GLU	B	903	20.387	39.361	16.065	1.00	39.59
ATOM	577	N	TYR	B	904	23.817	39.039	11.558	1.00	36.26
ATOM	578	CA	TYR	B	904	25.236	38.729	11.507	1.00	38.11
ATOM	579	C	TYR	B	904	25.928	39.016	12.842	1.00	36.13
ATOM	580	O	TYR	B	904	25.810	40.085	13.447	1.00	36.04
ATOM	581	CB	TYR	B	904	25.870	39.456	10.293	1.00	38.03
ATOM	582	CG	TYR	B	904	27.340	39.121	10.159	1.00	39.56
ATOM	583	CD1	TYR	B	904	27.790	37.827	9.900	1.00	40.02
ATOM	584	CD2	TYR	B	904	28.296	40.122	10.364	1.00	39.80
ATOM	585	CE1	TYR	B	904	29.134	37.532	9.822	1.00	40.07
ATOM	586	CE2	TYR	B	904	29.641	39.846	10.258	1.00	39.30
ATOM	587	CZ	TYR	B	904	30.043	38.571	9.994	1.00	38.67
ATOM	588	OH	TYR	B	904	31.395	38.341	9.943	1.00	42.02
ATOM	589	N	ALA	B	905	26.565	37.994	13.427	1.00	33.70
ATOM	590	CA	ALA	B	905	27.351	38.148	14.629	1.00	34.04
ATOM	591	C	ALA	B	905	28.807	38.331	14.173	1.00	34.59
ATOM	592	O	ALA	B	905	29.422	37.413	13.631	1.00	34.61
ATOM	593	CB	ALA	B	905	27.272	36.924	15.544	1.00	31.52
ATOM	594	N	PRO	B	906	29.362	39.523	14.313	1.00	37.23
ATOM	595	CA	PRO	B	906	30.702	39.735	13.790	1.00	36.90
ATOM	596	C	PRO	B	906	31.854	39.167	14.554	1.00	37.30
ATOM	597	O	PRO	B	906	32.998	39.226	14.071	1.00	37.05
ATOM	598	CB	PRO	B	906	30.757	41.248	13.601	1.00	38.72
ATOM	599	CG	PRO	B	906	29.641	41.840	14.378	1.00	39.46
ATOM	600	CD	PRO	B	906	28.736	40.738	14.854	1.00	35.60
ATOM	601	N	HIS	B	907	31.720	38.652	15.767	1.00	35.76
ATOM	602	CA	HIS	B	907	32.810	38.072	16.515	1.00	34.45
ATOM	603	C	HIS	B	907	32.768	36.551	16.532	1.00	33.29
ATOM	604	O	HIS	B	907	33.420	36.044	17.429	1.00	36.68
ATOM	605	CB	HIS	B	907	32.793	38.614	17.971	1.00	32.90
ATOM	606	CG	HIS	B	907	32.706	40.082	17.966	1.00	33.20
ATOM	607	ND1	HIS	B	907	33.802	40.846	17.590	1.00	35.03
ATOM	608	CD2	HIS	B	907	31.727	40.985	18.200	1.00	31.98
ATOM	609	CE1	HIS	B	907	33.497	42.128	17.610	1.00	33.06
ATOM	610	NE2	HIS	B	907	32.241	42.248	18.017	1.00	33.02
ATOM	611	N	GLY	B	908	32.021	35.804	15.757	1.00	30.48
ATOM	612	CA	GLY	B	908	32.010	34.380	15.765	1.00	32.68
ATOM	613	C	GLY	B	908	31.084	33.774	16.838	1.00	31.58
ATOM	614	O	GLY	B	908	30.218	34.407	17.431	1.00	28.30
ATOM	615	N	ASN	B	909	31.300	32.477	17.068	1.00	27.49
ATOM	616	CA	ASN	B	909	30.550	31.793	18.108	1.00	24.09
ATOM	617	C	ASN	B	909	31.321	32.036	19.407	1.00	25.93
ATOM	618	O	ASN	B	909	32.485	32.498	19.367	1.00	28.49
ATOM	619	CB	ASN	B	909	30.241	30.343	17.894	1.00	26.09
ATOM	620	CG	ASN	B	909	31.306	29.286	17.946	1.00	28.79
ATOM	621	OD1	ASN	B	909	31.088	28.055	17.867	1.00	30.89
ATOM	622	ND2	ASN	B	909	32.526	29.772	18.045	1.00	25.36

ATOM	623	N	LEU B 910	30.721	31.746	20.545	1.00	23.98
ATOM	624	CA	LEU B 910	31.369	32.013	21.809	1.00	24.27
ATOM	625	C	LEU B 910	32.494	31.025	22.149	1.00	28.34
ATOM	626	O	LEU B 910	33.475	31.482	22.740	1.00	28.22
ATOM	627	CB	LEU B 910	30.268	31.885	22.850	1.00	22.33
ATOM	628	CG	LEU B 910	30.701	31.957	24.327	1.00	23.69
ATOM	629	CD1	LEU B 910	31.394	33.213	24.683	1.00	22.29
ATOM	630	CD2	LEU B 910	29.417	31.790	25.166	1.00	21.67
ATOM	631	N	LEU B 911	32.290	29.750	21.805	1.00	27.95
ATOM	632	CA	LEU B 911	33.380	28.801	22.034	1.00	25.73
ATOM	633	C	LEU B 911	34.638	29.295	21.337	1.00	27.49
ATOM	634	O	LEU B 911	35.676	29.359	22.043	1.00	26.42
ATOM	635	CB	LEU B 911	33.003	27.396	21.533	1.00	27.05
ATOM	636	CG	LEU B 911	34.062	26.292	21.771	1.00	25.84
ATOM	637	CD1	LEU B 911	34.319	26.301	23.302	1.00	20.85
ATOM	638	CD2	LEU B 911	33.505	24.899	21.410	1.00	23.88
ATOM	639	N	ASP B 912	34.686	29.509	20.034	1.00	27.48
ATOM	640	CA	ASP B 912	35.832	30.077	19.341	1.00	30.26
ATOM	641	C	ASP B 912	36.323	31.426	19.869	1.00	31.88
ATOM	642	O	ASP B 912	37.540	31.676	19.938	1.00	29.65
ATOM	643	CB	ASP B 912	35.557	30.313	17.848	1.00	30.57
ATOM	644	CG	ASP B 912	35.339	29.102	16.995	1.00	34.53
ATOM	645	OD1	ASP B 912	34.882	29.274	15.841	1.00	37.84
ATOM	646	OD2	ASP B 912	35.663	27.975	17.416	1.00	37.21
ATOM	647	N	PHE B 913	35.440	32.298	20.355	1.00	31.78
ATOM	648	CA	PHE B 913	35.763	33.564	20.967	1.00	29.21
ATOM	649	C	PHE B 913	36.507	33.319	22.291	1.00	30.28
ATOM	650	O	PHE B 913	37.612	33.931	22.463	1.00	27.63
ATOM	651	CB	PHE B 913	34.591	34.492	21.208	1.00	27.45
ATOM	652	CG	PHE B 913	34.831	35.958	21.499	1.00	29.93
ATOM	653	CD1	PHE B 913	35.060	36.840	20.461	1.00	28.75
ATOM	654	CD2	PHE B 913	34.910	36.415	22.816	1.00	27.43
ATOM	655	CE1	PHE B 913	35.313	38.202	20.715	1.00	28.06
ATOM	656	CE2	PHE B 913	35.188	37.763	23.068	1.00	29.46
ATOM	657	CZ	PHE B 913	35.379	38.643	22.029	1.00	28.47
ATOM	658	N	LEU B 914	36.054	32.404	23.151	1.00	26.55
ATOM	659	CA	LEU B 914	36.844	32.188	24.365	1.00	31.20
ATOM	660	C	LEU B 914	38.154	31.425	24.075	1.00	30.42
ATOM	661	O	LEU B 914	39.065	31.539	24.890	1.00	29.64
ATOM	662	CB	LEU B 914	36.133	31.379	25.440	1.00	32.99
ATOM	663	CG	LEU B 914	34.718	31.897	25.858	1.00	32.39
ATOM	664	CD1	LEU B 914	33.745	30.794	26.190	1.00	31.43
ATOM	665	CD2	LEU B 914	34.981	32.805	27.062	1.00	27.44
ATOM	666	N	ARG B 915	38.196	30.595	23.029	1.00	28.43
ATOM	667	CA	ARG B 915	39.414	29.824	22.755	1.00	29.31
ATOM	668	C	ARG B 915	40.498	30.753	22.149	1.00	32.00
ATOM	669	O	ARG B 915	41.692	30.583	22.478	1.00	33.32
ATOM	670	CB	ARG B 915	39.157	28.572	21.911	1.00	25.22
ATOM	671	CG	ARG B 915	38.723	27.348	22.800	1.00	24.37
ATOM	672	CD	ARG B 915	38.161	26.209	21.957	1.00	24.35
ATOM	673	NE	ARG B 915	37.642	25.132	22.889	1.00	26.89
ATOM	674	CZ	ARG B 915	37.100	24.031	22.346	1.00	25.09
ATOM	675	NH1	ARG B 915	37.054	23.901	21.016	1.00	24.19
ATOM	676	NH2	ARG B 915	36.588	23.111	23.194	1.00	23.94
ATOM	677	N	LYS B 916	40.164	31.751	21.372	1.00	34.12
ATOM	678	CA	LYS B 916	40.980	32.736	20.705	1.00	35.63
ATOM	679	C	LYS B 916	41.664	33.693	21.683	1.00	36.01

FIG. 5L

ATOM	680	O	LYS	B	916	42.762	34.252	21.536	1.00	36.61
ATOM	681	CB	LYS	B	916	40.287	33.552	19.615	1.00	34.37
ATOM	682	CG	LYS	B	916	40.129	32.825	18.298	1.00	42.16
ATOM	683	CD	LYS	B	916	39.443	33.575	17.172	1.00	44.43
ATOM	684	CE	LYS	B	916	38.756	32.732	16.114	1.00	47.47
ATOM	685	NZ	LYS	B	916	37.371	33.261	15.814	1.00	51.77
ATOM	686	N	SER	B	917	40.991	33.857	22.786	1.00	33.46
ATOM	687	CA	SER	B	917	41.419	34.647	23.937	1.00	32.01
ATOM	688	C	SER	B	917	42.545	34.012	24.721	1.00	32.62
ATOM	689	O	SER	B	917	43.188	34.725	25.520	1.00	27.96
ATOM	690	CB	SER	B	917	40.117	34.800	24.689	1.00	31.09
ATOM	691	OG	SER	B	917	40.057	34.497	26.054	1.00	33.24
ATOM	692	N	ARG	B	918	42.926	32.735	24.574	1.00	33.26
ATOM	693	CA	ARG	B	918	43.911	32.087	25.401	1.00	29.88
ATOM	694	C	ARG	B	918	45.341	32.471	24.927	1.00	33.33
ATOM	695	O	ARG	B	918	46.072	31.782	24.226	1.00	34.36
ATOM	696	CB	ARG	B	918	43.750	30.570	25.487	1.00	30.84
ATOM	697	CG	ARG	B	918	42.350	30.118	25.969	1.00	31.53
ATOM	698	CD	ARG	B	918	42.301	28.655	26.234	1.00	31.59
ATOM	699	NE	ARG	B	918	41.373	27.771	26.776	1.00	30.40
ATOM	700	CZ	ARG	B	918	41.314	26.510	27.146	1.00	27.78
ATOM	701	NH1	ARG	B	918	42.579	25.901	27.032	1.00	24.30
ATOM	702	NH2	ARG	B	918	40.359	25.804	27.635	1.00	24.57
ATOM	703	N	VAL	B	919	45.792	33.639	25.388	1.00	29.19
ATOM	704	CA	VAL	B	919	46.914	34.362	24.991	1.00	31.89
ATOM	705	C	VAL	B	919	48.324	33.779	25.390	1.00	33.48
ATOM	706	O	VAL	B	919	49.318	34.428	25.239	1.00	42.15
ATOM	707	CB	VAL	B	919	47.064	35.854	25.366	1.00	30.88
ATOM	708	CG1	VAL	B	919	46.027	36.669	24.602	1.00	34.82
ATOM	709	CG2	VAL	B	919	46.881	36.061	26.852	1.00	31.88
ATOM	710	N	LEU	B	920	48.272	32.609	25.986	1.00	31.42
ATOM	711	CA	LEU	B	920	49.386	31.803	26.310	1.00	32.43
ATOM	712	C	LEU	B	920	49.646	30.949	25.049	1.00	33.59
ATOM	713	O	LEU	B	920	50.874	30.754	24.757	1.00	34.43
ATOM	714	CB	LEU	B	920	49.363	30.892	27.516	1.00	26.98
ATOM	715	CG	LEU	B	920	49.473	31.646	28.827	1.00	28.45
ATOM	716	CD1	LEU	B	920	49.060	30.712	29.911	1.00	24.11
ATOM	717	CD2	LEU	B	920	50.899	32.259	29.084	1.00	24.38
ATOM	718	N	GLU	B	921	48.560	30.587	24.414	1.00	33.03
ATOM	719	CA	GLU	B	921	48.691	29.839	23.163	1.00	34.88
ATOM	720	C	GLU	B	921	48.686	30.741	21.960	1.00	36.44
ATOM	721	O	GLU	B	921	49.468	30.532	21.028	1.00	37.60
ATOM	722	CB	GLU	B	921	47.526	28.797	23.034	1.00	36.48
ATOM	723	CG	GLU	B	921	47.367	28.228	21.636	1.00	39.16
ATOM	724	CD	GLU	B	921	46.213	27.255	21.414	1.00	43.37
ATOM	725	OE1	GLU	B	921	45.489	26.854	22.357	1.00	41.90
ATOM	726	OE2	GLU	B	921	46.044	26.848	20.222	1.00	42.19
ATOM	727	N	THR	B	922	47.772	31.738	21.886	1.00	33.22
ATOM	728	CA	THR	B	922	47.684	32.482	20.652	1.00	33.16
ATOM	729	C	THR	B	922	48.566	33.711	20.605	1.00	33.32
ATOM	730	O	THR	B	922	48.787	34.124	19.452	1.00	33.82
ATOM	731	CB	THR	B	922	46.212	32.897	20.346	1.00	33.96
ATOM	732	OG1	THR	B	922	45.814	33.744	21.415	1.00	33.38
ATOM	733	CG2	THR	B	922	45.288	31.667	20.363	1.00	35.79
ATOM	734	N	ASP	B	923	49.134	34.252	21.645	1.00	34.17
ATOM	735	CA	ASP	B	923	50.099	35.410	21.445	1.00	33.90
ATOM	736	C	ASP	B	923	50.855	35.464	22.736	1.00	31.06

FIG. 5M

ATOM	737	O	ASP	B	923	50.593	36.342	23.567	1.00	27.46
ATOM	738	CB	ASP	B	923	49.307	36.710	21.268	1.00	37.04
ATOM	739	CG	ASP	B	923	50.153	37.937	20.960	1.00	41.38
ATOM	740	OD1	ASP	B	923	49.577	39.035	20.699	1.00	39.51
ATOM	741	OD2	ASP	B	923	51.412	37.813	20.986	1.00	38.37
ATOM	742	N	PRO	B	924	51.732	34.505	23.057	1.00	30.87
ATOM	743	CA	PRO	B	924	52.373	34.348	24.339	1.00	29.10
ATOM	744	C	PRO	B	924	53.219	35.487	24.884	1.00	30.48
ATOM	745	O	PRO	B	924	53.451	35.658	26.081	1.00	36.16
ATOM	746	CB	PRO	B	924	53.266	33.088	24.160	1.00	29.12
ATOM	747	CG	PRO	B	924	53.404	32.976	22.696	1.00	30.23
ATOM	748	CD	PRO	B	924	52.076	33.382	22.137	1.00	31.39
ATOM	749	N	ALA	B	925	53.613	36.368	24.008	1.00	26.00
ATOM	750	CA	ALA	B	925	54.366	37.598	24.150	1.00	32.47
ATOM	751	C	ALA	B	925	53.543	38.653	24.869	1.00	29.57
ATOM	752	O	ALA	B	925	53.787	39.195	25.935	1.00	30.49
ATOM	753	CB	ALA	B	925	54.773	38.221	22.799	1.00	31.57
ATOM	754	N	PHE	B	926	52.319	38.825	24.295	1.00	29.73
ATOM	755	CA	PHE	B	926	51.269	39.710	24.838	1.00	29.93
ATOM	756	C	PHE	B	926	51.056	39.489	26.342	1.00	26.49
ATOM	757	O	PHE	B	926	50.877	40.391	27.189	1.00	33.60
ATOM	758	CB	PHE	B	926	49.990	39.510	24.004	1.00	33.75
ATOM	759	CG	PHE	B	926	48.853	40.282	24.610	1.00	35.41
ATOM	760	CD1	PHE	B	926	48.530	41.563	24.201	1.00	35.32
ATOM	761	CD2	PHE	B	926	48.148	39.708	25.665	1.00	35.43
ATOM	762	CE1	PHE	B	926	47.510	42.237	24.860	1.00	37.62
ATOM	763	CE2	PHE	B	926	47.135	40.390	26.312	1.00	40.82
ATOM	764	CZ	PHE	B	926	46.803	41.649	25.884	1.00	37.83
ATOM	765	N	ALA	B	927	50.917	38.202	26.616	1.00	30.01
ATOM	766	CA	ALA	B	927	50.632	37.486	27.815	1.00	28.56
ATOM	767	C	ALA	B	927	51.656	37.637	28.900	1.00	29.51
ATOM	768	O	ALA	B	927	51.289	37.839	30.056	1.00	30.25
ATOM	769	CB	ALA	B	927	50.513	35.973	27.565	1.00	32.88
ATOM	770	N	ILE	B	928	52.948	37.452	28.535	1.00	31.84
ATOM	771	CA	ILE	B	928	54.019	37.696	29.494	1.00	33.06
ATOM	772	C	ILE	B	928	54.111	39.221	29.662	1.00	31.39
ATOM	773	O	ILE	B	928	54.206	39.681	30.804	1.00	32.12
ATOM	774	CB	ILE	B	928	55.354	37.042	29.050	1.00	34.86
ATOM	775	CG1	ILE	B	928	56.448	37.311	30.077	1.00	36.35
ATOM	776	CG2	ILE	B	928	55.833	37.483	27.689	1.00	36.48
ATOM	777	CD1	ILE	B	928	56.235	36.372	31.274	1.00	40.48
ATOM	778	N	ALA	B	929	53.998	40.026	28.623	1.00	32.07
ATOM	779	CA	ALA	B	929	54.114	41.493	28.884	1.00	35.07
ATOM	780	C	ALA	B	929	52.935	42.038	29.650	1.00	32.88
ATOM	781	O	ALA	B	929	53.152	42.885	30.515	1.00	32.96
ATOM	782	CB	ALA	B	929	54.276	42.286	27.584	1.00	38.44
ATOM	783	N	ASN	B	930	51.737	41.363	29.538	1.00	32.01
ATOM	784	CA	ASN	B	930	50.624	41.923	30.307	1.00	32.62
ATOM	785	C	ASN	B	930	50.458	41.157	31.604	1.00	32.33
ATOM	786	O	ASN	B	930	49.549	41.509	32.315	1.00	30.28
ATOM	787	CB	ASN	B	930	49.305	41.975	29.564	1.00	30.21
ATOM	788	CG	ASN	B	930	49.462	43.166	28.612	1.00	34.16
ATOM	789	OD1	ASN	B	930	49.104	44.224	29.139	1.00	35.09
ATOM	790	ND2	ASN	B	930	49.997	42.925	27.434	1.00	33.29
ATOM	791	N	SER	B	931	51.284	40.126	31.740	1.00	31.40
ATOM	792	CA	SER	B	931	51.064	39.195	32.863	1.00	34.73
ATOM	793	C	SER	B	931	49.616	38.647	32.909	1.00	31.81

ATOM	794	O	SER	B	931	48.946	38.522	33.960	1.00	28.51
ATOM	795	CB	SER	B	931	51.539	39.966	34.083	1.00	36.38
ATOM	796	OG	SER	B	931	51.372	39.137	35.239	1.00	44.81
ATOM	797	N	THR	B	932	49.066	38.367	31.708	1.00	31.32
ATOM	798	CA	THR	B	932	47.681	37.822	31.741	1.00	33.33
ATOM	799	C	THR	B	932	47.532	36.490	31.036	1.00	31.10
ATOM	800	O	THR	B	932	48.276	36.141	30.127	1.00	30.68
ATOM	801	CB	THR	B	932	46.678	38.870	31.263	1.00	33.87
ATOM	802	OG1	THR	B	932	45.316	38.426	31.576	1.00	33.49
ATOM	803	CG2	THR	B	932	46.692	39.109	29.757	1.00	33.71
ATOM	804	N	ALA	B	933	46.529	35.668	31.389	1.00	31.61
ATOM	805	CA	ALA	B	933	46.226	34.431	30.705	1.00	29.07
ATOM	806	C	ALA	B	933	45.091	34.589	29.655	1.00	30.40
ATOM	807	O	ALA	B	933	44.908	33.676	28.853	1.00	28.66
ATOM	808	CB	ALA	B	933	45.737	33.378	31.703	1.00	27.24
ATOM	809	N	SER	B	934	44.450	35.779	29.587	1.00	26.77
ATOM	810	CA	SER	B	934	43.413	36.013	28.587	1.00	28.62
ATOM	811	C	SER	B	934	43.192	37.464	28.195	1.00	27.31
ATOM	812	O	SER	B	934	43.323	38.417	28.980	1.00	27.55
ATOM	813	CB	SER	B	934	42.064	35.455	29.162	1.00	26.81
ATOM	814	OG	SER	B	934	40.981	35.744	28.323	1.00	27.56
ATOM	815	N	THR	B	935	42.820	37.745	26.944	1.00	27.99
ATOM	816	CA	THR	B	935	42.439	39.110	26.578	1.00	29.68
ATOM	817	C	THR	B	935	41.160	39.524	27.282	1.00	31.68
ATOM	818	O	THR	B	935	40.842	40.718	27.320	1.00	33.62
ATOM	819	CB	THR	B	935	42.242	39.350	25.075	1.00	28.76
ATOM	820	OG1	THR	B	935	41.506	38.262	24.505	1.00	29.66
ATOM	821	CG2	THR	B	935	43.525	39.478	24.287	1.00	30.80
ATOM	822	N	LEU	B	936	40.343	38.579	27.771	1.00	30.00
ATOM	823	CA	LEU	B	936	39.018	38.902	28.323	1.00	31.45
ATOM	824	C	LEU	B	936	39.137	39.093	29.820	1.00	29.86
ATOM	825	O	LEU	B	936	39.947	38.339	30.364	1.00	28.85
ATOM	826	CB	LEU	B	936	38.171	37.634	28.127	1.00	35.21
ATOM	827	CG	LEU	B	936	37.312	37.342	26.944	1.00	38.52
ATOM	828	CD1	LEU	B	936	37.602	38.053	25.641	1.00	42.04
ATOM	829	CD2	LEU	B	936	37.181	35.833	26.689	1.00	40.21
ATOM	830	N	SER	B	937	38.381	39.888	30.508	1.00	28.66
ATOM	831	CA	SER	B	937	38.427	39.976	31.975	1.00	27.30
ATOM	832	C	SER	B	937	37.373	39.107	32.612	1.00	25.12
ATOM	833	O	SER	B	937	36.444	38.641	31.960	1.00	29.26
ATOM	834	CB	SER	B	937	38.164	41.408	32.478	1.00	28.29
ATOM	835	OG	SER	B	937	36.753	41.746	32.275	1.00	26.99
ATOM	836	N	SER	B	938	37.382	38.946	33.936	1.00	23.75
ATOM	837	CA	SER	B	938	36.444	38.301	34.738	1.00	25.14
ATOM	838	C	SER	B	938	34.982	38.781	34.508	1.00	29.67
ATOM	839	O	SER	B	938	33.973	38.052	34.324	1.00	28.12
ATOM	840	CB	SER	B	938	36.842	38.693	36.180	1.00	25.42
ATOM	841	OG	SER	B	938	35.935	37.879	36.971	1.00	31.24
ATOM	842	N	GLN	B	939	34.834	40.109	34.487	1.00	27.93
ATOM	843	CA	GLN	B	939	33.576	40.797	34.290	1.00	30.16
ATOM	844	C	GLN	B	939	33.036	40.463	32.911	1.00	26.11
ATOM	845	O	GLN	B	939	31.840	40.271	32.714	1.00	28.65
ATOM	846	CB	GLN	B	939	33.784	42.330	34.312	1.00	33.19
ATOM	847	CG	GLN	B	939	33.442	43.229	35.457	1.00	40.59
ATOM	848	CD	GLN	B	939	32.130	43.133	36.180	1.00	39.70
ATOM	849	OE1	GLN	B	939	31.005	43.468	35.831	1.00	47.06
ATOM	850	NE2	GLN	B	939	32.185	42.646	37.424	1.00	42.39

FIG. 50

ATOM	851	N	GLN	B	940	33.893	40.437	31.879	1.00	28.10
ATOM	852	CA	GLN	B	940	33.294	39.992	30.590	1.00	26.42
ATOM	853	C	GLN	B	940	32.792	38.510	30.608	1.00	27.93
ATOM	854	O	GLN	B	940	31.699	38.213	30.003	1.00	24.42
ATOM	855	CB	GLN	B	940	34.237	40.315	29.474	1.00	28.32
ATOM	856	CG	GLN	B	940	33.821	39.728	28.138	1.00	30.12
ATOM	857	CD	GLN	B	940	32.714	40.351	27.341	1.00	32.84
ATOM	858	OE1	GLN	B	940	32.980	40.952	26.293	1.00	32.97
ATOM	859	NE2	GLN	B	940	31.444	40.215	27.742	1.00	32.92
ATOM	860	N	LEU	B	941	33.469	37.651	31.370	1.00	26.91
ATOM	861	CA	LEU	B	941	32.909	36.258	31.443	1.00	28.19
ATOM	862	C	LEU	B	941	31.569	36.301	32.198	1.00	29.57
ATOM	863	O	LEU	B	941	30.678	35.590	31.730	1.00	30.43
ATOM	864	CB	LEU	B	941	33.906	35.296	32.049	1.00	25.27
ATOM	865	CG	LEU	B	941	35.315	35.323	31.415	1.00	32.42
ATOM	866	CD1	LEU	B	941	36.323	34.485	32.227	1.00	31.29
ATOM	867	CD2	LEU	B	941	35.341	34.767	30.010	1.00	31.88
ATOM	868	N	LEU	B	942	31.450	37.064	33.293	1.00	30.31
ATOM	869	CA	LEU	B	942	30.167	37.145	33.968	1.00	32.16
ATOM	870	C	LEU	B	942	29.036	37.749	33.115	1.00	31.83
ATOM	871	O	LEU	B	942	27.922	37.185	33.174	1.00	33.88
ATOM	872	CB	LEU	B	942	30.243	37.957	35.236	1.00	31.72
ATOM	873	CG	LEU	B	942	31.083	37.434	36.382	1.00	33.04
ATOM	874	CD1	LEU	B	942	31.284	38.550	37.417	1.00	33.30
ATOM	875	CD2	LEU	B	942	30.573	36.187	36.999	1.00	35.60
ATOM	876	N	HIS	B	943	29.333	38.722	32.292	1.00	30.14
ATOM	877	CA	HIS	B	943	28.489	39.305	31.307	1.00	32.55
ATOM	878	C	HIS	B	943	27.988	38.261	30.293	1.00	33.04
ATOM	879	O	HIS	B	943	26.773	38.281	29.997	1.00	29.13
ATOM	880	CB	HIS	B	943	29.051	40.525	30.513	1.00	31.92
ATOM	881	CG	HIS	B	943	28.919	41.826	31.219	1.00	34.62
ATOM	882	ND1	HIS	B	943	29.954	42.688	31.481	1.00	36.03
ATOM	883	CD2	HIS	B	943	27.832	42.442	31.778	1.00	38.05
ATOM	884	CE1	HIS	B	943	29.547	43.737	32.168	1.00	35.60
ATOM	885	NE2	HIS	B	943	28.245	43.626	32.354	1.00	37.32
ATOM	886	N	PHE	B	944	28.860	37.419	29.710	1.00	30.43
ATOM	887	CA	PHE	B	944	28.322	36.430	28.793	1.00	30.42
ATOM	888	C	PHE	B	944	27.361	35.447	29.480	1.00	28.35
ATOM	889	O	PHE	B	944	26.297	35.095	28.948	1.00	27.55
ATOM	890	CB	PHE	B	944	29.414	35.601	28.129	1.00	29.40
ATOM	891	CG	PHE	B	944	30.259	36.326	27.143	1.00	28.28
ATOM	892	CD1	PHE	B	944	31.639	36.118	27.152	1.00	28.85
ATOM	893	CD2	PHE	B	944	29.764	37.193	26.200	1.00	27.36
ATOM	894	CE1	PHE	B	944	32.429	36.783	26.230	1.00	31.22
ATOM	895	CE2	PHE	B	944	30.528	37.861	25.279	1.00	30.76
ATOM	896	CZ	PHE	B	944	31.863	37.640	25.305	1.00	29.54
ATOM	897	N	ALA	B	945	27.661	35.064	30.707	1.00	28.20
ATOM	898	CA	ALA	B	945	26.737	34.232	31.526	1.00	27.06
ATOM	899	C	ALA	B	945	25.389	34.896	31.781	1.00	28.16
ATOM	900	O	ALA	B	945	24.305	34.272	31.603	1.00	29.72
ATOM	901	CB	ALA	B	945	27.424	33.982	32.882	1.00	22.24
ATOM	902	N	ALA	B	946	25.348	36.185	32.154	1.00	28.40
ATOM	903	CA	ALA	B	946	24.058	36.906	32.424	1.00	26.80
ATOM	904	C	ALA	B	946	23.326	37.071	31.128	1.00	26.73
ATOM	905	O	ALA	B	946	22.095	36.826	30.960	1.00	33.16
ATOM	906	CB	ALA	B	946	24.422	38.268	33.049	1.00	27.29
ATOM	907	N	ASP	B	947	24.021	37.501	30.077	1.00	25.12

FIG. 5P

ATOM	908	CA	ASP	B	947	23.361	37.562	28.793	1.00	27.64
ATOM	909	C	ASP	B	947	22.653	36.217	28.522	1.00	30.15
ATOM	910	O	ASP	B	947	21.423	36.331	28.285	1.00	32.77
ATOM	911	CB	ASP	B	947	24.158	37.947	27.594	1.00	32.32
ATOM	912	CG	ASP	B	947	24.798	39.318	27.538	1.00	37.39
ATOM	913	OD1	ASP	B	947	24.327	40.283	28.209	1.00	38.95
ATOM	914	OD2	ASP	B	947	25.817	39.462	26.816	1.00	38.99
ATOM	915	N	VAL	B	948	23.225	35.043	28.511	1.00	24.93
ATOM	916	CA	VAL	B	948	22.519	33.824	28.235	1.00	26.37
ATOM	917	C	VAL	B	948	21.319	33.657	29.150	1.00	26.38
ATOM	918	O	VAL	B	948	20.273	33.241	28.688	1.00	28.00
ATOM	919	CB	VAL	B	948	23.423	32.575	28.375	1.00	23.63
ATOM	920	CG1	VAL	B	948	22.711	31.247	28.218	1.00	28.41
ATOM	921	CG2	VAL	B	948	24.500	32.621	27.306	1.00	24.29
ATOM	922	N	ALA	B	949	21.496	33.853	30.472	1.00	25.90
ATOM	923	CA	ALA	B	949	20.489	33.633	31.449	1.00	24.76
ATOM	924	C	ALA	B	949	19.254	34.514	31.245	1.00	29.82
ATOM	925	O	ALA	B	949	18.125	33.995	31.478	1.00	29.12
ATOM	926	CB	ALA	B	949	21.105	33.945	32.833	1.00	21.23
ATOM	927	N	ARG	B	950	19.483	35.753	30.814	1.00	29.05
ATOM	928	CA	ARG	B	950	18.417	36.711	30.563	1.00	29.74
ATOM	929	C	ARG	B	950	17.681	36.245	29.315	1.00	30.35
ATOM	930	O	ARG	B	950	16.454	36.156	29.291	1.00	32.30
ATOM	931	CB	ARG	B	950	18.943	38.135	30.331	1.00	29.04
ATOM	932	CG	ARG	B	950	17.857	39.209	30.253	1.00	29.74
ATOM	933	CD	ARG	B	950	18.484	40.540	29.840	1.00	33.11
ATOM	934	NE	ARG	B	950	19.702	40.789	30.623	1.00	36.26
ATOM	935	CZ	ARG	B	950	20.973	41.064	30.349	1.00	36.47
ATOM	936	NH1	ARG	B	950	21.905	41.281	31.276	1.00	34.51
ATOM	937	NH2	ARG	B	950	21.378	41.083	29.088	1.00	37.31
ATOM	938	N	GLY	B	951	18.419	35.817	28.306	1.00	29.52
ATOM	939	CA	GLY	B	951	17.811	35.222	27.135	1.00	30.22
ATOM	940	C	GLY	B	951	16.981	34.005	27.518	1.00	31.96
ATOM	941	O	GLY	B	951	15.802	33.895	27.083	1.00	30.42
ATOM	942	N	MET	B	952	17.505	33.082	28.335	1.00	31.58
ATOM	943	CA	MET	B	952	16.833	31.858	28.668	1.00	31.52
ATOM	944	C	MET	B	952	15.593	32.060	29.545	1.00	31.14
ATOM	945	O	MET	B	952	14.692	31.277	29.453	1.00	32.05
ATOM	946	CB	MET	B	952	17.728	30.817	29.348	1.00	32.91
ATOM	947	CG	MET	B	952	18.601	29.963	28.470	1.00	28.12
ATOM	948	SD	MET	B	952	17.803	29.220	27.056	1.00	28.47
ATOM	949	CE	MET	B	952	16.601	28.118	27.850	1.00	24.09
ATOM	950	N	ASP	B	953	15.540	32.991	30.425	1.00	33.12
ATOM	951	CA	ASP	B	953	14.479	33.295	31.364	1.00	35.52
ATOM	952	C	ASP	B	953	13.331	33.873	30.536	1.00	34.51
ATOM	953	O	ASP	B	953	12.167	33.463	30.579	1.00	34.88
ATOM	954	CB	ASP	B	953	14.959	34.196	32.470	1.00	37.38
ATOM	955	CG	ASP	B	953	13.886	35.033	33.182	1.00	38.60
ATOM	956	OD1	ASP	B	953	13.235	34.579	34.136	1.00	38.16
ATOM	957	OD2	ASP	B	953	13.774	36.209	32.830	1.00	39.51
ATOM	958	N	TYR	B	954	13.741	34.680	29.561	1.00	34.22
ATOM	959	CA	TYR	B	954	12.764	35.208	28.602	1.00	33.92
ATOM	960	C	TYR	B	954	12.083	34.027	27.920	1.00	35.03
ATOM	961	O	TYR	B	954	10.854	33.911	27.879	1.00	33.83
ATOM	962	CB	TYR	B	954	13.457	36.158	27.672	1.00	36.04
ATOM	963	CG	TYR	B	954	12.621	36.621	26.523	1.00	40.14
ATOM	964	CD1	TYR	B	954	11.489	37.372	26.834	1.00	42.51

FIG. 5Q

ATOM	965	CD2	TYR	B	954	12.873	36.322	25.202	1.00	40.08
ATOM	966	CE1	TYR	B	954	10.587	37.819	25.869	1.00	45.17
ATOM	967	CE2	TYR	B	954	12.012	36.762	24.225	1.00	44.28
ATOM	968	CZ	TYR	B	954	10.893	37.541	24.548	1.00	45.99
ATOM	969	OH	TYR	B	954	10.043	37.968	23.564	1.00	46.72
ATOM	970	N	LEU	B	955	12.809	33.080	27.399	1.00	34.55
ATOM	971	CA	LEU	B	955	12.388	31.912	26.704	1.00	34.31
ATOM	972	C	LEU	B	955	11.690	30.956	27.654	1.00	32.95
ATOM	973	O	LEU	B	955	10.537	30.633	27.336	1.00	36.79
ATOM	974	CB	LEU	B	955	13.431	31.053	26.006	1.00	34.82
ATOM	975	CG	LEU	B	955	14.032	31.673	24.757	1.00	30.87
ATOM	976	CD1	LEU	B	955	15.304	30.976	24.341	1.00	31.55
ATOM	977	CD2	LEU	B	955	13.075	31.726	23.592	1.00	32.89
ATOM	978	N	SER	B	956	12.231	30.620	28.798	1.00	33.38
ATOM	979	CA	SER	B	956	11.489	29.672	29.609	1.00	34.02
ATOM	980	C	SER	B	956	10.214	30.243	30.247	1.00	34.18
ATOM	981	O	SER	B	956	9.393	29.419	30.652	1.00	30.24
ATOM	982	CB	SER	B	956	12.469	29.126	30.630	1.00	33.64
ATOM	983	OG	SER	B	956	12.613	30.134	31.586	1.00	37.17
ATOM	984	N	GLN	B	957	10.032	31.530	30.438	1.00	32.94
ATOM	985	CA	GLN	B	957	8.852	32.137	31.059	1.00	37.57
ATOM	986	C	GLN	B	957	7.675	32.048	30.084	1.00	36.65
ATOM	987	O	GLN	B	957	6.518	31.962	30.443	1.00	36.69
ATOM	988	CB	GLN	B	957	9.101	33.516	31.671	1.00	39.36
ATOM	989	CG	GLN	B	957	9.819	33.491	33.028	1.00	43.44
ATOM	990	CD	GLN	B	957	10.305	34.801	33.581	1.00	47.63
ATOM	991	OE1	GLN	B	957	10.420	35.138	34.789	1.00	48.94
ATOM	992	NE2	GLN	B	957	10.736	35.802	32.807	1.00	50.75
ATOM	993	N	LYS	B	958	7.937	31.933	28.792	1.00	37.29
ATOM	994	CA	LYS	B	958	7.068	31.649	27.696	1.00	36.90
ATOM	995	C	LYS	B	958	6.830	30.166	27.402	1.00	39.87
ATOM	996	O	LYS	B	958	6.248	29.735	26.407	1.00	41.16
ATOM	997	CB	LYS	B	958	7.554	32.393	26.439	1.00	40.75
ATOM	998	CG	LYS	B	958	7.237	33.882	26.545	1.00	42.57
ATOM	999	CD	LYS	B	958	7.853	34.666	25.399	1.00	44.52
ATOM	1000	CE	LYS	B	958	6.950	35.852	25.045	1.00	49.59
ATOM	1001	NZ	LYS	B	958	7.755	36.850	24.277	1.00	50.56
ATOM	1002	N	GLN	B	959	7.238	29.272	28.275	1.00	38.89
ATOM	1003	CA	GLN	B	959	7.191	27.826	28.340	1.00	39.77
ATOM	1004	C	GLN	B	959	7.985	27.154	27.246	1.00	36.45
ATOM	1005	O	GLN	B	959	7.889	25.977	26.904	1.00	34.64
ATOM	1006	CB	GLN	B	959	5.729	27.298	28.353	1.00	42.27
ATOM	1007	CG	GLN	B	959	5.062	27.411	29.706	1.00	47.02
ATOM	1008	CD	GLN	B	959	3.550	27.270	29.700	1.00	52.44
ATOM	1009	OE1	GLN	B	959	2.905	27.301	30.787	1.00	54.64
ATOM	1010	NE2	GLN	B	959	2.888	27.133	28.539	1.00	51.33
ATOM	1011	N	PHE	B	960	8.932	27.911	26.701	1.00	35.89
ATOM	1012	CA	PHE	B	960	9.764	27.490	25.601	1.00	34.12
ATOM	1013	C	PHE	B	960	11.017	26.758	26.168	1.00	34.10
ATOM	1014	O	PHE	B	960	11.310	27.045	27.320	1.00	36.77
ATOM	1015	CB	PHE	B	960	10.127	28.752	24.850	1.00	38.30
ATOM	1016	CG	PHE	B	960	9.381	29.131	23.626	1.00	37.64
ATOM	1017	CD1	PHE	B	960	8.691	30.350	23.577	1.00	39.17
ATOM	1018	CD2	PHE	B	960	9.322	28.313	22.534	1.00	37.83
ATOM	1019	CE1	PHE	B	960	7.970	30.753	22.460	1.00	36.50
ATOM	1020	CE2	PHE	B	960	8.612	28.711	21.415	1.00	38.89
ATOM	1021	CZ	PHE	B	960	7.938	29.930	21.372	1.00	38.28

FIG. 5R

ATOM	1022	N	ILE	B	961	11.301	25.645	25.515	1.00	32.04
ATOM	1023	CA	ILE	B	961	12.386	24.751	25.913	1.00	35.73
ATOM	1024	C	ILE	B	961	13.444	24.628	24.815	1.00	35.82
ATOM	1025	O	ILE	B	961	13.170	24.025	23.764	1.00	36.60
ATOM	1026	CB	ILE	B	961	11.866	23.322	26.185	1.00	37.85
ATOM	1027	CG1	ILE	B	961	10.658	23.219	27.079	1.00	39.27
ATOM	1028	CG2	ILE	B	961	12.985	22.443	26.741	1.00	41.20
ATOM	1029	CD1	ILE	B	961	10.666	23.505	28.545	1.00	39.36
ATOM	1030	N	HIS	B	962	14.751	24.959	25.030	1.00	33.60
ATOM	1031	CA	HIS	B	962	15.736	24.996	23.975	1.00	31.29
ATOM	1032	C	HIS	B	962	16.435	23.705	23.604	1.00	30.82
ATOM	1033	O	HIS	B	962	16.658	23.371	22.425	1.00	29.73
ATOM	1034	CB	HIS	B	962	16.674	26.099	24.539	1.00	31.33
ATOM	1035	CG	HIS	B	962	17.589	26.596	23.457	1.00	33.97
ATOM	1036	ND1	HIS	B	962	17.135	26.808	22.169	1.00	33.33
ATOM	1037	CD2	HIS	B	962	18.913	26.881	23.499	1.00	33.27
ATOM	1038	CE1	HIS	B	962	18.200	27.242	21.492	1.00	35.73
ATOM	1039	NE2	HIS	B	962	19.289	27.260	22.251	1.00	29.66
ATOM	1040	N	ARG	B	963	16.968	23.006	24.598	1.00	30.47
ATOM	1041	CA	ARG	B	963	17.746	21.769	24.471	1.00	33.00
ATOM	1042	C	ARG	B	963	19.194	21.923	23.997	1.00	36.77
ATOM	1043	O	ARG	B	963	19.889	20.887	24.004	1.00	39.62
ATOM	1044	CB	ARG	B	963	17.204	20.679	23.551	1.00	32.77
ATOM	1045	CG	ARG	B	963	15.815	20.172	23.935	1.00	31.62
ATOM	1046	CD	ARG	B	963	15.128	19.404	22.847	1.00	31.53
ATOM	1047	NE	ARG	B	963	15.025	19.871	21.521	1.00	33.88
ATOM	1048	CZ	ARG	B	963	15.726	19.662	20.419	1.00	37.97
ATOM	1049	NH1	ARG	B	963	16.808	18.841	20.421	1.00	37.50
ATOM	1050	NH2	ARG	B	963	15.341	20.285	19.289	1.00	37.35
ATOM	1051	N	ASN	B	964	19.655	23.009	23.398	1.00	36.17
ATOM	1052	CA	ASN	B	964	20.974	23.021	22.816	1.00	38.69
ATOM	1053	C	ASN	B	964	21.926	24.070	23.372	1.00	36.17
ATOM	1054	O	ASN	B	964	22.772	24.513	22.610	1.00	37.84
ATOM	1055	CB	ASN	B	964	20.798	23.344	21.298	1.00	41.85
ATOM	1056	CG	ASN	B	964	20.079	22.173	20.634	1.00	46.78
ATOM	1057	OD1	ASN	B	964	20.319	21.037	21.043	1.00	49.94
ATOM	1058	ND2	ASN	B	964	19.184	22.496	19.688	1.00	48.13
ATOM	1059	N	LEU	B	965	21.795	24.534	24.570	1.00	32.14
ATOM	1060	CA	LEU	B	965	22.546	25.569	25.189	1.00	33.80
ATOM	1061	C	LEU	B	965	23.994	25.064	25.398	1.00	36.44
ATOM	1062	O	LEU	B	965	24.144	24.390	26.421	1.00	40.41
ATOM	1063	CB	LEU	B	965	22.086	25.960	26.578	1.00	31.51
ATOM	1064	CG	LEU	B	965	20.940	26.943	26.863	1.00	30.06
ATOM	1065	CD1	LEU	B	965	20.731	26.975	28.363	1.00	26.70
ATOM	1066	CD2	LEU	B	965	21.491	28.298	26.403	1.00	29.20
ATOM	1067	N	ALA	B	966	24.919	25.275	24.490	1.00	31.71
ATOM	1068	CA	ALA	B	966	26.340	24.956	24.701	1.00	29.62
ATOM	1069	C	ALA	B	966	27.144	26.139	24.175	1.00	27.97
ATOM	1070	O	ALA	B	966	26.676	26.823	23.232	1.00	24.99
ATOM	1071	CB	ALA	B	966	26.737	23.681	23.960	1.00	24.98
ATOM	1072	N	ALA	B	967	28.451	26.232	24.492	1.00	28.41
ATOM	1073	CA	ALA	B	967	29.236	27.348	23.991	1.00	25.71
ATOM	1074	C	ALA	B	967	29.357	27.432	22.481	1.00	28.11
ATOM	1075	O	ALA	B	967	29.291	28.561	21.897	1.00	26.71
ATOM	1076	CB	ALA	B	967	30.515	27.596	24.725	1.00	28.93
ATOM	1077	N	ARG	B	968	29.406	26.364	21.727	1.00	30.03
ATOM	1078	CA	ARG	B	968	29.407	26.477	20.257	1.00	30.09

FIG. 5S

ATOM	1079	C	ARG	B	968	28.100	27.003	19.677	1.00	30.62
ATOM	1080	O	ARG	B	968	28.131	27.362	18.476	1.00	31.68
ATOM	1081	CB	ARG	B	968	29.753	25.111	19.610	1.00	29.15
ATOM	1082	CG	ARG	B	968	28.695	24.044	19.886	1.00	31.62
ATOM	1083	CD	ARG	B	968	28.941	22.658	19.226	1.00	35.47
ATOM	1084	NE	ARG	B	968	27.817	21.807	19.703	1.00	38.33
ATOM	1085	CZ	ARG	B	968	27.827	21.154	20.851	1.00	40.05
ATOM	1086	NH1	ARG	B	968	28.897	21.164	21.633	1.00	42.72
ATOM	1087	NH2	ARG	B	968	26.834	20.421	21.322	1.00	43.32
ATOM	1088	N	ASN	B	969	26.979	27.025	20.436	1.00	28.92
ATOM	1089	CA	ASN	B	969	25.710	27.429	19.810	1.00	29.20
ATOM	1090	C	ASN	B	969	25.291	28.803	20.297	1.00	30.35
ATOM	1091	O	ASN	B	969	24.086	29.145	20.204	1.00	30.32
ATOM	1092	CB	ASN	B	969	24.598	26.375	20.098	1.00	25.04
ATOM	1093	CG	ASN	B	969	24.914	25.020	19.495	1.00	30.26
ATOM	1094	OD1	ASN	B	969	25.378	24.869	18.361	1.00	32.57
ATOM	1095	ND2	ASN	B	969	24.648	23.886	20.172	1.00	28.51
ATOM	1096	N	ILE	B	970	26.257	29.496	20.910	1.00	27.55
ATOM	1097	CA	ILE	B	970	26.015	30.841	21.418	1.00	28.82
ATOM	1098	C	ILE	B	970	26.802	31.795	20.505	1.00	29.55
ATOM	1099	O	ILE	B	970	27.963	31.487	20.196	1.00	27.59
ATOM	1100	CB	ILE	B	970	26.412	31.038	22.895	1.00	26.22
ATOM	1101	CG1	ILE	B	970	25.618	30.198	23.893	1.00	25.70
ATOM	1102	CG2	ILE	B	970	26.312	32.536	23.261	1.00	21.48
ATOM	1103	CD1	ILE	B	970	24.088	30.263	23.734	1.00	23.69
ATOM	1104	N	LEU	B	971	26.208	32.904	20.028	1.00	29.96
ATOM	1105	CA	LEU	B	971	26.961	33.826	19.172	1.00	30.19
ATOM	1106	C	LEU	B	971	27.438	35.090	19.845	1.00	31.70
ATOM	1107	O	LEU	B	971	26.784	35.584	20.761	1.00	33.46
ATOM	1108	CB	LEU	B	971	26.085	34.128	17.930	1.00	30.67
ATOM	1109	CG	LEU	B	971	25.855	32.975	16.964	1.00	34.15
ATOM	1110	CD1	LEU	B	971	24.695	33.281	15.982	1.00	33.06
ATOM	1111	CD2	LEU	B	971	27.122	32.553	16.185	1.00	30.70
ATOM	1112	N	VAL	B	972	28.541	35.731	19.447	1.00	30.83
ATOM	1113	CA	VAL	B	972	29.044	36.982	20.037	1.00	32.48
ATOM	1114	C	VAL	B	972	28.758	38.104	19.005	1.00	30.36
ATOM	1115	O	VAL	B	972	29.405	38.186	17.951	1.00	31.08
ATOM	1116	CB	VAL	B	972	30.521	36.984	20.420	1.00	32.58
ATOM	1117	CG1	VAL	B	972	30.930	38.281	21.136	1.00	34.22
ATOM	1118	CG2	VAL	B	972	30.871	35.785	21.333	1.00	31.21
ATOM	1119	N	GLY	B	973	27.711	38.847	19.310	1.00	30.33
ATOM	1120	CA	GLY	B	973	27.207	39.802	18.315	1.00	29.88
ATOM	1121	C	GLY	B	973	27.727	41.204	18.479	1.00	32.70
ATOM	1122	O	GLY	B	973	28.585	41.451	19.329	1.00	31.01
ATOM	1123	N	GLU	B	974	27.145	42.135	17.747	1.00	34.65
ATOM	1124	CA	GLU	B	974	27.522	43.527	17.855	1.00	33.72
ATOM	1125	C	GLU	B	974	27.649	43.930	19.302	1.00	33.97
ATOM	1126	O	GLU	B	974	26.870	43.530	20.180	1.00	30.31
ATOM	1127	CB	GLU	B	974	26.420	44.367	17.187	1.00	40.43
ATOM	1128	CG	GLU	B	974	26.557	44.283	15.649	1.00	48.26
ATOM	1129	CD	GLU	B	974	26.317	45.679	15.071	1.00	54.12
ATOM	1130	OE1	GLU	B	974	25.119	46.052	15.074	1.00	56.77
ATOM	1131	OE2	GLU	B	974	27.258	46.414	14.674	1.00	56.47
ATOM	1132	N	ASN	B	975	28.679	44.730	19.612	1.00	32.99
ATOM	1133	CA	ASN	B	975	28.909	45.235	20.945	1.00	32.09
ATOM	1134	C	ASN	B	975	29.202	44.081	21.877	1.00	32.69
ATOM	1135	O	ASN	B	975	29.082	44.240	23.098	1.00	33.59

FIG. 5T

ATOM	1136	CB	ASN	B	975	27.642	46.019	21.385	1.00	36.61
ATOM	1137	CG	ASN	B	975	27.446	47.285	20.540	1.00	37.11
ATOM	1138	OD1	ASN	B	975	26.276	47.739	20.363	1.00	39.26
ATOM	1139	ND2	ASN	B	975	28.530	47.826	20.042	1.00	29.86
ATOM	1140	N	TYR	B	976	29.715	42.945	21.379	1.00	32.96
ATOM	1141	CA	TYR	B	976	29.974	41.815	22.291	1.00	33.87
ATOM	1142	C	TYR	B	976	28.745	41.291	22.977	1.00	33.96
ATOM	1143	O	TYR	B	976	28.952	40.845	24.142	1.00	38.50
ATOM	1144	CB	TYR	B	976	31.090	42.145	23.319	1.00	32.57
ATOM	1145	CG	TYR	B	976	32.316	42.635	22.562	1.00	34.93
ATOM	1146	CD1	TYR	B	976	32.643	43.977	22.488	1.00	34.96
ATOM	1147	CD2	TYR	B	976	33.064	41.750	21.796	1.00	36.25
ATOM	1148	CE1	TYR	B	976	33.734	44.404	21.765	1.00	36.57
ATOM	1149	CE2	TYR	B	976	34.151	42.185	21.066	1.00	37.74
ATOM	1150	CZ	TYR	B	976	34.469	43.524	21.027	1.00	38.58
ATOM	1151	OH	TYR	B	976	35.544	43.988	20.318	1.00	41.08
ATOM	1152	N	VAL	B	977	27.498	41.318	22.583	1.00	33.38
ATOM	1153	CA	VAL	B	977	26.363	40.804	23.354	1.00	30.29
ATOM	1154	C	VAL	B	977	26.160	39.324	23.034	1.00	28.06
ATOM	1155	O	VAL	B	977	26.157	38.975	21.853	1.00	30.23
ATOM	1156	CB	VAL	B	977	25.135	41.674	23.014	1.00	29.39
ATOM	1157	CG1	VAL	B	977	23.846	41.027	23.499	1.00	28.20
ATOM	1158	CG2	VAL	B	977	25.284	43.038	23.718	1.00	31.72
ATOM	1159	N	ALA	B	978	26.159	38.459	24.028	1.00	27.76
ATOM	1160	CA	ALA	B	978	25.975	37.006	23.681	1.00	28.79
ATOM	1161	C	ALA	B	978	24.563	36.847	23.132	1.00	31.90
ATOM	1162	O	ALA	B	978	23.647	37.514	23.577	1.00	30.56
ATOM	1163	CB	ALA	B	978	26.186	36.192	24.917	1.00	25.90
ATOM	1164	N	LYS	B	979	24.330	36.043	22.103	1.00	33.62
ATOM	1165	CA	LYS	B	979	23.070	35.784	21.463	1.00	31.66
ATOM	1166	C	LYS	B	979	22.780	34.287	21.336	1.00	31.79
ATOM	1167	O	LYS	B	979	23.561	33.490	20.808	1.00	29.59
ATOM	1168	CB	LYS	B	979	23.102	36.390	20.030	1.00	34.05
ATOM	1169	CG	LYS	B	979	22.883	37.917	20.237	1.00	38.30
ATOM	1170	CD	LYS	B	979	23.149	38.766	19.049	1.00	36.22
ATOM	1171	CE	LYS	B	979	23.157	40.252	19.366	1.00	39.70
ATOM	1172	NZ	LYS	B	979	21.788	40.833	19.313	1.00	39.24
ATOM	1173	N	ILE	B	980	21.643	33.866	21.839	1.00	29.92
ATOM	1174	CA	ILE	B	980	21.279	32.444	21.718	1.00	29.31
ATOM	1175	C	ILE	B	980	20.877	32.083	20.290	1.00	32.94
ATOM	1176	O	ILE	B	980	20.093	32.771	19.620	1.00	34.86
ATOM	1177	CB	ILE	B	980	20.142	32.123	22.676	1.00	27.87
ATOM	1178	CG1	ILE	B	980	20.564	32.314	24.120	1.00	29.18
ATOM	1179	CG2	ILE	B	980	19.778	30.614	22.519	1.00	32.98
ATOM	1180	CD1	ILE	B	980	19.477	32.141	25.157	1.00	26.99
ATOM	1181	N	ALA	B	981	21.425	30.940	19.843	1.00	33.63
ATOM	1182	CA	ALA	B	981	21.100	30.397	18.542	1.00	34.72
ATOM	1183	C	ALA	B	981	20.872	28.883	18.597	1.00	36.94
ATOM	1184	O	ALA	B	981	20.993	28.205	19.630	1.00	36.37
ATOM	1185	CB	ALA	B	981	22.158	30.764	17.532	1.00	32.74
ATOM	1186	N	ASP	B	982	20.702	28.316	17.416	1.00	38.89
ATOM	1187	CA	ASP	B	982	20.540	26.898	17.122	1.00	38.46
ATOM	1188	C	ASP	B	982	19.195	26.448	17.713	1.00	37.99
ATOM	1189	O	ASP	B	982	19.092	25.674	18.675	1.00	36.61
ATOM	1190	CB	ASP	B	982	21.703	26.016	17.541	1.00	40.25
ATOM	1191	CG	ASP	B	982	21.452	24.552	17.184	1.00	43.41
ATOM	1192	OD1	ASP	B	982	20.728	24.230	16.205	1.00	46.24

FIG. 5U

ATOM	1193	OD2	ASP	B	982	21.281	23.629	17.877	1.00	42.63
ATOM	1194	N	PHE	B	983	18.165	27.008	17.126	1.00	36.77
ATOM	1195	CA	PHE	B	983	16.782	26.774	17.503	1.00	41.16
ATOM	1196	C	PHE	B	983	16.065	25.567	16.890	1.00	42.48
ATOM	1197	O	PHE	B	983	16.087	25.257	15.684	1.00	43.89
ATOM	1198	CB	PHE	B	983	15.964	28.059	17.163	1.00	39.87
ATOM	1199	CG	PHE	B	983	16.280	29.135	18.179	1.00	39.48
ATOM	1200	CD1	PHE	B	983	15.940	28.923	19.504	1.00	38.68
ATOM	1201	CD2	PHE	B	983	16.957	30.289	17.825	1.00	39.97
ATOM	1202	CE1	PHE	B	983	16.251	29.809	20.491	1.00	37.05
ATOM	1203	CE2	PHE	B	983	17.257	31.221	18.816	1.00	40.42
ATOM	1204	CZ	PHE	B	983	16.906	30.993	20.135	1.00	39.41
ATOM	1205	N	GLY	B	984	15.346	24.852	17.733	1.00	41.51
ATOM	1206	CA	GLY	B	984	14.461	23.724	17.265	1.00	41.21
ATOM	1207	C	GLY	B	984	13.535	23.685	18.500	1.00	40.75
ATOM	1208	O	GLY	B	984	13.678	22.812	19.368	1.00	40.87
ATOM	1209	N	LEU	B	985	12.781	24.779	18.612	1.00	38.40
ATOM	1210	CA	LEU	B	985	12.020	25.010	19.826	1.00	38.54
ATOM	1211	C	LEU	B	985	10.844	24.053	20.021	1.00	39.23
ATOM	1212	O	LEU	B	985	10.331	23.451	19.099	1.00	39.81
ATOM	1213	CB	LEU	B	985	11.597	26.477	19.879	1.00	38.29
ATOM	1214	CG	LEU	B	985	12.703	27.505	20.071	1.00	39.62
ATOM	1215	CD1	LEU	B	985	12.112	28.913	19.963	1.00	41.67
ATOM	1216	CD2	LEU	B	985	13.378	27.375	21.450	1.00	40.64
ATOM	1217	N	SER	B	986	10.420	23.923	21.268	1.00	38.75
ATOM	1218	CA	SER	B	986	9.258	23.124	21.640	1.00	41.57
ATOM	1219	C	SER	B	986	8.618	23.946	22.764	1.00	41.04
ATOM	1220	O	SER	B	986	9.376	24.681	23.389	1.00	40.97
ATOM	1221	CB	SER	B	986	9.623	21.781	22.276	1.00	41.12
ATOM	1222	OG	SER	B	986	10.132	20.965	21.268	1.00	44.70
ATOM	1223	N	ARG	B	987	7.306	23.872	22.881	1.00	41.47
ATOM	1224	CA	ARG	B	987	6.579	24.634	23.849	1.00	39.96
ATOM	1225	C	ARG	B	987	5.664	23.672	24.592	1.00	39.46
ATOM	1226	O	ARG	B	987	4.928	22.897	24.001	1.00	40.85
ATOM	1227	CB	ARG	B	987	5.759	25.671	23.100	1.00	42.69
ATOM	1228	CG	ARG	B	987	5.518	26.881	23.980	1.00	43.46
ATOM	1229	CD	ARG	B	987	4.820	27.932	23.102	1.00	47.12
ATOM	1230	NE	ARG	B	987	4.503	29.062	23.969	1.00	48.45
ATOM	1231	CZ	ARG	B	987	4.042	30.245	23.498	1.00	49.30
ATOM	1232	NH1	ARG	B	987	3.859	30.446	22.195	1.00	47.75
ATOM	1233	NH2	ARG	B	987	3.820	31.126	24.461	1.00	47.10
ATOM	1234	N	GLY	B	988	5.803	23.678	25.895	1.00	36.84
ATOM	1235	CA	GLY	B	988	5.310	22.780	26.860	1.00	37.53
ATOM	1236	C	GLY	B	988	6.133	22.613	28.131	1.00	39.84
ATOM	1237	O	GLY	B	988	7.113	23.319	28.413	1.00	37.68
ATOM	1238	N	GLN	B	989	5.621	21.679	28.931	1.00	37.98
ATOM	1239	CA	GLN	B	989	6.211	21.351	30.208	1.00	36.52
ATOM	1240	C	GLN	B	989	7.342	20.344	29.982	1.00	36.26
ATOM	1241	O	GLN	B	989	8.364	20.451	30.678	1.00	35.23
ATOM	1242	CB	GLN	B	989	5.134	20.856	31.154	1.00	36.36
ATOM	1243	CG	GLN	B	989	5.676	20.186	32.391	1.00	39.62
ATOM	1244	CD	GLN	B	989	4.653	19.836	33.425	1.00	39.25
ATOM	1245	OE1	GLN	B	989	4.232	20.788	34.082	1.00	42.73
ATOM	1246	NE2	GLN	B	989	4.255	18.604	33.639	1.00	40.97
ATOM	1247	N	GLU	B	990	7.214	19.459	28.997	1.00	33.95
ATOM	1248	CA	GLU	B	990	8.362	18.545	28.745	1.00	32.76
ATOM	1249	C	GLU	B	990	8.318	18.162	27.281	1.00	31.62

FIG. 5V

ATOM	1250	O	GLU	B	990	7.134	18.267	26.782	1.00	35.90
ATOM	1251	CB	GLU	B	990	8.324	17.321	29.615	1.00	32.06
ATOM	1252	CG	GLU	B	990	7.034	16.491	29.549	1.00	34.29
ATOM	1253	CD	GLU	B	990	5.855	16.986	30.361	1.00	35.18
ATOM	1254	OE1	GLU	B	990	4.741	17.354	29.866	1.00	31.61
ATOM	1255	OE2	GLU	B	990	5.907	17.055	31.606	1.00	37.46
ATOM	1256	N	VAL	B	991	9.245	17.586	26.636	1.00	28.59
ATOM	1257	CA	VAL	B	991	9.254	17.187	25.250	1.00	27.10
ATOM	1258	C	VAL	B	991	10.294	16.035	25.123	1.00	34.31
ATOM	1259	O	VAL	B	991	11.499	16.047	25.461	1.00	34.01
ATOM	1260	CB	VAL	B	991	9.566	18.341	24.297	1.00	27.78
ATOM	1261	CG1	VAL	B	991	10.981	18.939	24.577	1.00	28.52
ATOM	1262	CG2	VAL	B	991	9.531	17.878	22.827	1.00	26.55
ATOM	1263	N	TYR	B	992	9.815	15.116	24.284	1.00	33.22
ATOM	1264	CA	TYR	B	992	10.510	13.950	23.872	1.00	35.07
ATOM	1265	C	TYR	B	992	11.168	14.196	22.521	1.00	36.09
ATOM	1266	O	TYR	B	992	10.453	14.723	21.653	1.00	37.35
ATOM	1267	CB	TYR	B	992	9.504	12.750	23.851	1.00	32.12
ATOM	1268	CG	TYR	B	992	10.187	11.588	23.154	1.00	34.00
ATOM	1269	CD1	TYR	B	992	10.952	10.664	23.855	1.00	35.23
ATOM	1270	CD2	TYR	B	992	10.065	11.491	21.767	1.00	34.41
ATOM	1271	CE1	TYR	B	992	11.597	9.629	23.205	1.00	34.80
ATOM	1272	CE2	TYR	B	992	10.706	10.464	21.115	1.00	35.88
ATOM	1273	CZ	TYR	B	992	11.471	9.575	21.830	1.00	37.31
ATOM	1274	OH	TYR	B	992	12.090	8.582	21.090	1.00	41.58
ATOM	1275	N	VAL	B	993	12.465	13.922	22.409	1.00	35.09
ATOM	1276	CA	VAL	B	993	13.166	14.093	21.148	1.00	40.55
ATOM	1277	C	VAL	B	993	14.192	12.937	21.077	1.00	44.20
ATOM	1278	O	VAL	B	993	14.924	12.698	22.027	1.00	41.10
ATOM	1279	CB	VAL	B	993	14.027	15.345	20.884	1.00	40.80
ATOM	1280	CG1	VAL	B	993	14.377	15.434	19.397	1.00	41.00
ATOM	1281	CG2	VAL	B	993	13.444	16.675	21.308	1.00	40.65
ATOM	1282	N	LYS	B	994	14.248	12.280	19.929	1.00	52.91
ATOM	1283	CA	LYS	B	994	15.228	11.218	19.681	1.00	59.67
ATOM	1284	C	LYS	B	994	16.314	11.668	18.722	1.00	63.50
ATOM	1285	O	LYS	B	994	15.968	12.346	17.752	1.00	65.43
ATOM	1286	CB	LYS	B	994	14.452	10.051	19.050	1.00	62.12
ATOM	1287	CG	LYS	B	994	15.258	9.165	18.114	1.00	64.47
ATOM	1288	CD	LYS	B	994	14.523	7.917	17.676	1.00	66.81
ATOM	1289	CE	LYS	B	994	14.741	6.737	18.627	1.00	69.22
ATOM	1290	NZ	LYS	B	994	16.113	6.131	18.446	1.00	70.28
ATOM	1291	N	LYS	B	995	17.568	11.244	18.841	1.00	68.11
ATOM	1292	CA	LYS	B	995	18.698	11.497	17.964	1.00	69.33
ATOM	1293	C	LYS	B	995	19.277	12.900	17.869	1.00	71.04
ATOM	1294	CB	LYS	B	995	18.387	11.058	16.520	1.00	68.75
ATOM	1295	N	THR	B	996	19.210	13.731	18.891	1.00	72.92
ATOM	1296	CA	THR	B	996	19.849	15.039	18.958	1.00	74.27
ATOM	1297	C	THR	B	996	18.897	16.170	18.571	1.00	74.88
ATOM	1298	O	THR	B	996	17.742	15.867	18.197	1.00	75.62
ATOM	1299	CB	THR	B	996	21.108	15.075	18.098	1.00	74.16
TER										
ATOM	1300	N	LEU	C	1000	24.923	13.250	19.201	1.00	61.56
ATOM	1301	CA	LEU	C	1000	24.606	13.627	20.610	1.00	60.45
ATOM	1302	C	LEU	C	1000	25.273	14.888	21.132	1.00	59.31
ATOM	1303	O	LEU	C	1000	25.926	15.737	20.498	1.00	61.19
ATOM	1304	CB	LEU	C	1000	25.085	12.439	21.459	1.00	62.33
ATOM	1305	N	PRO	C	1001	25.106	15.086	22.450	1.00	55.81

FIG. 5W

ATOM	1306	CA	PRO	C1001	25.717	16.238	23.164	1.00	47.68
ATOM	1307	C	PRO	C1001	25.633	15.865	24.622	1.00	42.57
ATOM	1308	O	PRO	C1001	25.066	16.507	25.497	1.00	42.56
ATOM	1309	CB	PRO	C1001	25.055	17.514	22.761	1.00	49.13
ATOM	1310	N	VAL	C1002	26.137	14.628	24.881	1.00	39.19
ATOM	1311	CA	VAL	C1002	26.105	13.982	26.180	1.00	36.21
ATOM	1312	C	VAL	C1002	26.526	14.731	27.414	1.00	32.43
ATOM	1313	O	VAL	C1002	25.981	14.707	28.510	1.00	29.30
ATOM	1314	CB	VAL	C1002	27.129	12.774	26.075	1.00	38.41
ATOM	1315	CG1	VAL	C1002	27.304	12.077	27.400	1.00	36.91
ATOM	1316	CG2	VAL	C1002	26.315	11.872	25.131	1.00	39.50
ATOM	1317	N	ARG	C1003	27.699	15.354	27.317	1.00	35.49
ATOM	1318	CA	ARG	C1003	28.454	16.101	28.310	1.00	34.85
ATOM	1319	C	ARG	C1003	27.745	17.378	28.731	1.00	32.80
ATOM	1320	O	ARG	C1003	28.073	18.089	29.675	1.00	33.09
ATOM	1321	CB	ARG	C1003	29.877	16.407	27.775	1.00	35.57
ATOM	1322	CG	ARG	C1003	30.017	15.726	26.418	1.00	40.79
ATOM	1323	CD	ARG	C1003	31.524	15.638	26.082	1.00	42.74
ATOM	1324	NE	ARG	C1003	32.199	15.018	27.219	1.00	46.61
ATOM	1325	CZ	ARG	C1003	33.482	14.536	26.897	1.00	42.40
ATOM	1326	NH1	ARG	C1003	33.675	14.646	25.606	1.00	44.69
ATOM	1327	NH2	ARG	C1003	34.058	13.991	27.899	1.00	41.82
ATOM	1328	N	TRP	C1004	26.753	17.765	27.983	1.00	31.57
ATOM	1329	CA	TRP	C1004	25.743	18.792	28.171	1.00	32.26
ATOM	1330	C	TRP	C1004	24.352	18.357	28.588	1.00	33.31
ATOM	1331	O	TRP	C1004	23.571	19.223	29.047	1.00	32.82
ATOM	1332	CB	TRP	C1004	25.513	19.633	26.877	1.00	31.61
ATOM	1333	CG	TRP	C1004	26.794	20.424	26.649	1.00	29.75
ATOM	1334	CD1	TRP	C1004	27.065	21.659	27.174	1.00	33.83
ATOM	1335	CD2	TRP	C1004	27.885	20.016	25.845	1.00	30.53
ATOM	1336	NE1	TRP	C1004	28.350	22.036	26.758	1.00	30.12
ATOM	1337	CE2	TRP	C1004	28.838	21.058	25.939	1.00	32.87
ATOM	1338	CE3	TRP	C1004	28.284	18.907	25.081	1.00	31.33
ATOM	1339	CZ2	TRP	C1004	30.114	21.052	25.322	1.00	31.29
ATOM	1340	CZ3	TRP	C1004	29.523	18.911	24.457	1.00	31.61
ATOM	1341	CH2	TRP	C1004	30.442	19.974	24.537	1.00	31.26
ATOM	1342	N	MET	C1005	24.039	17.058	28.523	1.00	31.05
ATOM	1343	CA	MET	C1005	22.691	16.644	28.871	1.00	30.92
ATOM	1344	C	MET	C1005	22.482	16.372	30.342	1.00	31.46
ATOM	1345	O	MET	C1005	23.344	15.779	30.955	1.00	30.88
ATOM	1346	CB	MET	C1005	22.425	15.401	28.027	1.00	35.15
ATOM	1347	CG	MET	C1005	22.250	15.671	26.542	1.00	35.78
ATOM	1348	SD	MET	C1005	22.331	14.145	25.574	1.00	43.66
ATOM	1349	CE	MET	C1005	20.582	13.671	25.658	1.00	39.42
ATOM	1350	N	ALA	C1006	21.331	16.767	30.898	1.00	30.39
ATOM	1351	CA	ALA	C1006	20.980	16.384	32.257	1.00	32.23
ATOM	1352	C	ALA	C1006	20.903	14.819	32.255	1.00	29.50
ATOM	1353	O	ALA	C1006	20.820	14.243	31.191	1.00	25.95
ATOM	1354	CB	ALA	C1006	19.558	16.827	32.686	1.00	32.19
ATOM	1355	N	ILE	C1007	21.063	14.271	33.415	1.00	28.66
ATOM	1356	CA	ILE	C1007	20.991	12.831	33.717	1.00	34.31
ATOM	1357	C	ILE	C1007	19.626	12.254	33.361	1.00	32.33
ATOM	1358	O	ILE	C1007	19.539	11.314	32.569	1.00	34.27
ATOM	1359	CB	ILE	C1007	21.316	12.831	35.238	1.00	36.74
ATOM	1360	CG1	ILE	C1007	22.831	12.539	35.418	1.00	40.16
ATOM	1361	CG2	ILE	C1007	20.535	11.850	36.027	1.00	41.55
ATOM	1362	CD1	ILE	C1007	23.298	12.738	36.843	1.00	39.53

FIG. 5X

ATOM	1363	N	GLU	C1008	18.515	12.879	33.668	1.00	32.21
ATOM	1364	CA	GLU	C1008	17.179	12.414	33.238	1.00	30.51
ATOM	1365	C	GLU	C1008	17.097	12.390	31.725	1.00	30.14
ATOM	1366	C	GLU	C1008	16.588	11.399	31.127	1.00	30.02
ATOM	1367	CB	GLU	C1008	16.079	13.201	33.887	1.00	32.29
ATOM	1368	CG	GLU	C1008	15.861	14.623	33.271	1.00	31.03
ATOM	1369	CD	GLU	C1008	16.672	15.611	34.070	1.00	30.62
ATOM	1370	OE1	GLU	C1008	17.610	15.181	34.800	1.00	33.04
ATOM	1371	OE2	GLU	C1008	16.405	16.824	34.011	1.00	33.30
ATOM	1372	N	SER	C1009	17.652	13.397	31.054	1.00	28.64
ATOM	1373	CA	SER	C1009	17.665	13.395	29.574	1.00	27.96
ATOM	1374	C	SER	C1009	18.581	12.320	29.008	1.00	32.36
ATOM	1375	O	SER	C1009	18.258	11.867	27.889	1.00	33.49
ATOM	1376	CB	SER	C1009	18.120	14.740	29.001	1.00	27.04
ATOM	1377	OG	SER	C1009	17.266	15.856	29.232	1.00	29.52
ATOM	1378	N	LEU	C1010	19.732	11.948	29.646	1.00	30.58
ATOM	1379	CA	LEU	C1010	20.458	10.834	29.043	1.00	33.82
ATOM	1380	C	LEU	C1010	19.587	9.543	29.184	1.00	34.58
ATOM	1381	O	LEU	C1010	19.600	8.647	28.340	1.00	33.77
ATOM	1382	CB	LEU	C1010	21.835	10.478	29.678	1.00	34.39
ATOM	1383	CG	LEU	C1010	22.839	11.659	29.618	1.00	34.04
ATOM	1384	CD1	LEU	C1010	23.989	11.636	30.582	1.00	35.06
ATOM	1385	CD2	LEU	C1010	23.324	11.698	28.183	1.00	34.32
ATOM	1386	N	ASN	C1011	18.894	9.423	30.317	1.00	34.50
ATOM	1387	CA	ASN	C1011	18.175	8.188	30.585	1.00	39.53
ATOM	1388	C	ASN	C1011	16.867	8.049	29.814	1.00	39.46
ATOM	1389	O	ASN	C1011	16.521	6.887	29.507	1.00	41.72
ATOM	1390	CB	ASN	C1011	17.744	7.990	32.055	1.00	37.12
ATOM	1391	CG	ASN	C1011	18.994	7.594	32.849	1.00	40.42
ATOM	1392	OD1	ASN	C1011	19.913	7.055	32.211	1.00	41.43
ATOM	1393	ND2	ASN	C1011	18.990	7.876	34.135	1.00	37.03
ATOM	1394	N	TYR	C1012	16.144	9.174	29.765	1.00	36.32
ATOM	1395	CA	TYR	C1012	14.765	9.067	29.205	1.00	33.71
ATOM	1396	C	TYR	C1012	14.644	9.864	27.929	1.00	37.07
ATOM	1397	O	TYR	C1012	13.431	9.936	27.557	1.00	39.06
ATOM	1398	CB	TYR	C1012	13.779	9.722	30.189	1.00	25.11
ATOM	1399	CG	TYR	C1012	13.979	9.247	31.601	1.00	26.79
ATOM	1400	CD1	TYR	C1012	13.915	10.061	32.704	1.00	28.02
ATOM	1401	CD2	TYR	C1012	14.199	7.868	31.824	1.00	29.96
ATOM	1402	CE1	TYR	C1012	14.075	9.560	33.984	1.00	31.07
ATOM	1403	CE2	TYR	C1012	14.378	7.325	33.070	1.00	30.68
ATOM	1404	CZ	TYR	C1012	14.310	8.194	34.126	1.00	32.85
ATOM	1405	OH	TYR	C1012	14.494	7.677	35.423	1.00	38.60
ATOM	1406	N	SER	C1013	15.568	10.695	27.480	1.00	35.61
ATOM	1407	CA	SER	C1013	15.244	11.547	26.340	1.00	36.12
ATOM	1408	C	SER	C1013	14.080	12.522	26.555	1.00	31.92
ATOM	1409	O	SER	C1013	13.533	12.997	25.558	1.00	29.49
ATOM	1410	CB	SER	C1013	15.021	10.764	25.075	1.00	38.37
ATOM	1411	OG	SER	C1013	16.000	9.929	24.605	1.00	39.85
ATOM	1412	N	VAL	C1014	13.848	12.926	27.798	1.00	34.71
ATOM	1413	CA	VAL	C1014	12.887	13.999	28.005	1.00	34.17
ATOM	1414	C	VAL	C1014	13.761	15.212	28.406	1.00	32.14
ATOM	1415	O	VAL	C1014	14.764	15.102	29.061	1.00	31.92
ATOM	1416	CB	VAL	C1014	11.803	13.647	29.007	1.00	35.91
ATOM	1417	CG1	VAL	C1014	10.773	14.771	28.958	1.00	35.03
ATOM	1418	CG2	VAL	C1014	11.129	12.316	28.672	1.00	35.03
ATOM	1419	N	TYR	C1015	13.255	16.377	27.994	1.00	33.31

ATOM	1420	CA	TYR	C1015	13.917	17.662	28.222	1.00	29.96
ATOM	1421	C	TYR	C1015	12.870	18.627	28.713	1.00	32.82
ATOM	1422	O	TYR	C1015	11.635	18.497	28.361	1.00	33.09
ATOM	1423	CB	TYR	C1015	14.268	18.208	26.817	1.00	31.34
ATOM	1424	CG	TYR	C1015	15.273	17.339	26.106	1.00	32.85
ATOM	1425	CD1	TYR	C1015	14.953	16.293	25.270	1.00	33.14
ATOM	1426	CD2	TYR	C1015	16.625	17.556	26.338	1.00	33.80
ATOM	1427	CE1	TYR	C1015	15.892	15.497	24.664	1.00	36.71
ATOM	1428	CE2	TYR	C1015	17.623	16.791	25.745	1.00	36.63
ATOM	1429	CZ	TYR	C1015	17.249	15.758	24.895	1.00	36.99
ATOM	1430	OH	TYR	C1015	18.233	15.005	24.325	1.00	37.59
ATOM	1431	N	THR	C1016	13.210	19.409	29.691	1.00	29.91
ATOM	1432	CA	THR	C1016	12.342	20.393	30.312	1.00	30.08
ATOM	1433	C	THR	C1016	13.109	21.700	30.459	1.00	33.68
ATOM	1434	O	THR	C1016	14.307	21.752	30.085	1.00	32.46
ATOM	1435	CB	THR	C1016	11.986	19.882	31.717	1.00	31.45
ATOM	1436	OG1	THR	C1016	13.149	19.778	32.540	1.00	31.21
ATOM	1437	CG2	THR	C1016	11.332	18.415	31.720	1.00	29.42
ATOM	1438	N	THR	C1017	12.509	22.699	31.141	1.00	31.49
ATOM	1439	CA	THR	C1017	13.301	23.863	31.536	1.00	32.10
ATOM	1440	C	THR	C1017	14.367	23.447	32.536	1.00	33.86
ATOM	1441	O	THR	C1017	15.480	24.004	32.588	1.00	31.99
ATOM	1442	CB	THR	C1017	12.396	25.033	32.078	1.00	32.15
ATOM	1443	OG1	THR	C1017	11.836	25.456	30.829	1.00	32.91
ATOM	1444	CG2	THR	C1017	13.152	26.192	32.675	1.00	30.94
ATOM	1445	N	ASN	C1018	14.062	22.468	33.403	1.00	32.36
ATOM	1446	CA	ASN	C1018	15.020	21.997	34.372	1.00	34.23
ATOM	1447	C	ASN	C1018	16.208	21.329	33.647	1.00	33.65
ATOM	1448	O	ASN	C1018	17.326	21.560	34.163	1.00	32.63
ATOM	1449	CB	ASN	C1018	14.563	21.089	35.519	1.00	33.92
ATOM	1450	CG	ASN	C1018	13.478	21.750	36.390	1.00	36.18
ATOM	1451	OD1	ASN	C1018	13.561	22.943	36.772	1.00	33.93
ATOM	1452	ND2	ASN	C1018	12.400	20.983	36.687	1.00	31.82
ATOM	1453	N	SER	C1019	16.007	20.738	32.468	1.00	30.11
ATOM	1454	CA	SER	C1019	17.216	20.101	31.865	1.00	31.68
ATOM	1455	C	SER	C1019	18.016	21.121	31.069	1.00	30.62
ATOM	1456	O	SER	C1019	19.237	21.110	30.787	1.00	25.61
ATOM	1457	CB	SER	C1019	16.668	18.883	31.150	1.00	29.04
ATOM	1458	OG	SER	C1019	16.208	19.177	29.829	1.00	30.35
ATOM	1459	N	ASP	C1020	17.331	22.228	30.738	1.00	30.23
ATOM	1460	CA	ASP	C1020	17.923	23.429	30.164	1.00	27.36
ATOM	1461	C	ASP	C1020	18.880	24.034	31.183	1.00	26.47
ATOM	1462	O	ASP	C1020	19.935	24.477	30.766	1.00	28.27
ATOM	1463	CB	ASP	C1020	16.986	24.536	29.714	1.00	28.00
ATOM	1464	CG	ASP	C1020	16.480	24.298	28.328	1.00	28.71
ATOM	1465	OD1	ASP	C1020	16.969	23.343	27.647	1.00	31.13
ATOM	1466	OD2	ASP	C1020	15.583	24.984	27.876	1.00	32.14
ATOM	1467	N	VAL	C1021	18.502	24.085	32.455	1.00	26.65
ATOM	1468	CA	VAL	C1021	19.328	24.627	33.497	1.00	26.02
ATOM	1469	C	VAL	C1021	20.546	23.742	33.781	1.00	27.12
ATOM	1470	O	VAL	C1021	21.575	24.333	34.098	1.00	23.97
ATOM	1471	CB	VAL	C1021	18.525	24.925	34.779	1.00	27.32
ATOM	1472	CG1	VAL	C1021	19.464	25.263	35.929	1.00	25.33
ATOM	1473	CG2	VAL	C1021	17.590	26.138	34.626	1.00	29.37
ATOM	1474	N	TRP	C1022	20.461	22.409	33.671	1.00	25.32
ATOM	1475	CA	TRP	C1022	21.679	21.587	33.868	1.00	23.28
ATOM	1476	C	TRP	C1022	22.664	21.958	32.796	1.00	23.00

FIG. 5Z

ATOM	1477	O	TRP	C1022	23.835	22.338	32.917	1.00	25.36
ATOM	1478	CB	TRP	C1022	21.248	20.096	33.625	1.00	25.77
ATOM	1479	CG	TRP	C1022	22.434	19.150	33.646	1.00	27.35
ATOM	1480	CD1	TRP	C1022	23.411	18.987	32.695	1.00	26.63
ATOM	1481	CD2	TRP	C1022	22.685	18.200	34.675	1.00	28.39
ATOM	1482	NE1	TRP	C1022	24.267	18.008	33.079	1.00	29.90
ATOM	1483	CE2	TRP	C1022	23.840	17.481	34.300	1.00	30.24
ATOM	1484	CE3	TRP	C1022	22.041	17.867	35.866	1.00	30.30
ATOM	1485	CZ2	TRP	C1022	24.394	16.485	35.090	1.00	32.33
ATOM	1486	CZ3	TRP	C1022	22.563	16.816	36.624	1.00	31.39
ATOM	1487	CH2	TRP	C1022	23.718	16.151	36.243	1.00	32.10
ATOM	1488	N	SER	C1023	22.207	21.928	31.529	1.00	21.23
ATOM	1489	CA	SER	C1023	23.068	22.354	30.379	1.00	22.80
ATOM	1490	C	SER	C1023	23.618	23.745	30.495	1.00	27.97
ATOM	1491	O	SER	C1023	24.829	24.031	30.146	1.00	23.26
ATOM	1492	CB	SER	C1023	22.108	21.769	29.326	1.00	24.28
ATOM	1493	OG	SER	C1023	21.977	22.454	28.131	1.00	34.21
ATOM	1494	N	TYR	C1024	22.810	24.769	30.968	1.00	24.68
ATOM	1495	CA	TYR	C1024	23.395	26.101	31.223	1.00	25.91
ATOM	1496	C	TYR	C1024	24.614	26.083	32.155	1.00	28.55
ATOM	1497	O	TYR	C1024	25.582	26.856	32.091	1.00	26.16
ATOM	1498	CB	TYR	C1024	22.317	27.041	31.808	1.00	23.53
ATOM	1499	CG	TYR	C1024	22.904	28.385	32.225	1.00	23.34
ATOM	1500	CD1	TYR	C1024	22.931	29.409	31.328	1.00	21.89
ATOM	1501	CD2	TYR	C1024	23.322	28.564	33.537	1.00	21.62
ATOM	1502	CE1	TYR	C1024	23.498	30.640	31.655	1.00	24.95
ATOM	1503	CE2	TYR	C1024	23.929	29.791	33.858	1.00	25.56
ATOM	1504	CZ	TYR	C1024	23.957	30.795	32.941	1.00	24.77
ATOM	1505	OH	TYR	C1024	24.513	32.006	33.282	1.00	29.84
ATOM	1506	N	GLY	C1025	24.559	25.263	33.180	1.00	31.16
ATOM	1507	CA	GLY	C1025	25.499	24.901	34.180	1.00	28.63
ATOM	1508	C	GLY	C1025	26.812	24.444	33.475	1.00	29.18
ATOM	1509	O	GLY	C1025	27.826	24.973	33.911	1.00	25.38
ATOM	1510	N	VAL	C1026	26.724	23.628	32.431	1.00	30.48
ATOM	1511	CA	VAL	C1026	27.848	23.171	31.665	1.00	30.49
ATOM	1512	C	VAL	C1026	28.404	24.335	30.867	1.00	30.61
ATOM	1513	O	VAL	C1026	29.622	24.566	30.796	1.00	31.75
ATOM	1514	CB	VAL	C1026	27.598	21.959	30.748	1.00	29.54
ATOM	1515	CG1	VAL	C1026	28.867	21.451	30.040	1.00	26.68
ATOM	1516	CG2	VAL	C1026	26.960	20.808	31.527	1.00	28.00
ATOM	1517	N	LEU	C1027	27.539	25.107	30.208	1.00	29.76
ATOM	1518	CA	LEU	C1027	27.925	26.331	29.524	1.00	27.25
ATOM	1519	C	LEU	C1027	28.729	27.263	30.410	1.00	25.12
ATOM	1520	O	LEU	C1027	29.764	27.833	30.030	1.00	27.00
ATOM	1521	CB	LEU	C1027	26.664	27.044	28.959	1.00	27.55
ATOM	1522	CG	LEU	C1027	26.904	28.561	28.667	1.00	27.68
ATOM	1523	CD1	LEU	C1027	27.658	28.914	27.434	1.00	28.77
ATOM	1524	CD2	LEU	C1027	25.485	29.174	28.511	1.00	29.96
ATOM	1525	N	LEU	C1028	28.311	27.500	31.665	1.00	27.12
ATOM	1526	CA	LEU	C1028	28.994	28.386	32.576	1.00	26.05
ATOM	1527	C	LEU	C1028	30.399	27.853	32.836	1.00	28.29
ATOM	1528	O	LEU	C1028	31.296	28.666	32.888	1.00	27.74
ATOM	1529	CB	LEU	C1028	28.123	28.576	33.809	1.00	24.95
ATOM	1530	CG	LEU	C1028	28.601	29.349	34.990	1.00	26.00
ATOM	1531	CD1	LEU	C1028	28.932	30.805	34.567	1.00	26.51
ATOM	1532	CD2	LEU	C1028	27.771	29.411	36.264	1.00	23.62
ATOM	1533	N	TRP	C1029	30.569	26.514	32.998	1.00	27.52

FIG. 5AA

ATOM	1534	CA	TRP	C1029	31.811	25.818	33.200	1.00	25.28
ATOM	1535	C	TRP	C1029	32.677	26.052	31.992	1.00	24.21
ATOM	1536	O	TRP	C1029	33.809	26.411	32.199	1.00	28.34
ATOM	1537	CB	TRP	C1029	31.604	24.291	33.488	1.00	25.52
ATOM	1538	CG	TRP	C1029	32.875	23.609	33.873	1.00	23.89
ATOM	1539	CD1	TRP	C1029	33.316	23.467	35.159	1.00	23.77
ATOM	1540	CD2	TRP	C1029	33.901	23.125	33.013	1.00	25.22
ATOM	1541	NE1	TRP	C1029	34.566	22.870	35.125	1.00	28.07
ATOM	1542	CE2	TRP	C1029	34.922	22.645	33.819	1.00	27.51
ATOM	1543	CE3	TRP	C1029	34.013	23.005	31.620	1.00	27.28
ATOM	1544	CZ2	TRP	C1029	36.095	21.998	33.349	1.00	30.61
ATOM	1545	CZ3	TRP	C1029	35.169	22.378	31.126	1.00	30.99
ATOM	1546	CH2	TRP	C1029	36.195	21.931	31.972	1.00	29.91
ATOM	1547	N	GLU	C1030	32.196	26.006	30.773	1.00	22.75
ATOM	1548	CA	GLU	C1030	32.865	26.380	29.590	1.00	24.64
ATOM	1549	C	GLU	C1030	33.291	27.882	29.553	1.00	23.46
ATOM	1550	O	GLU	C1030	34.433	28.114	29.047	1.00	23.61
ATOM	1551	CB	GLU	C1030	32.036	26.144	28.339	1.00	22.23
ATOM	1552	CG	GLU	C1030	31.853	24.671	28.076	1.00	27.85
ATOM	1553	CD	GLU	C1030	30.969	24.399	26.881	1.00	33.40
ATOM	1554	OE1	GLU	C1030	29.767	24.531	27.111	1.00	33.08
ATOM	1555	OE2	GLU	C1030	31.477	24.088	25.792	1.00	37.59
ATOM	1556	N	ILE	C1031	32.413	28.784	30.027	1.00	20.93
ATOM	1557	CA	ILE	C1031	32.888	30.190	29.987	1.00	23.32
ATOM	1558	C	ILE	C1031	34.099	30.417	30.881	1.00	24.20
ATOM	1559	O	ILE	C1031	35.125	31.060	30.547	1.00	25.10
ATOM	1560	CB	ILE	C1031	31.720	31.156	30.365	1.00	22.53
ATOM	1561	CG1	ILE	C1031	30.622	31.066	29.330	1.00	24.20
ATOM	1562	CG2	ILE	C1031	32.262	32.584	30.449	1.00	25.77
ATOM	1563	CD1	ILE	C1031	29.254	31.567	29.766	1.00	24.02
ATOM	1564	N	VAL	C1032	34.002	30.128	32.180	1.00	23.96
ATOM	1565	CA	VAL	C1032	34.923	30.263	33.255	1.00	28.42
ATOM	1566	C	VAL	C1032	36.251	29.547	32.943	1.00	31.87
ATOM	1567	O	VAL	C1032	37.324	30.118	33.157	1.00	31.88
ATOM	1568	CB	VAL	C1032	34.229	29.636	34.479	1.00	31.74
ATOM	1569	CG1	VAL	C1032	35.145	28.990	35.490	1.00	35.56
ATOM	1570	CG2	VAL	C1032	33.241	30.562	35.210	1.00	29.88
ATOM	1571	N	SER	C1033	36.236	28.433	32.262	1.00	29.60
ATOM	1572	CA	SER	C1033	37.352	27.612	31.846	1.00	29.62
ATOM	1573	C	SER	C1033	37.900	28.101	30.520	1.00	30.68
ATOM	1574	O	SER	C1033	38.900	27.598	30.046	1.00	30.21
ATOM	1575	CB	SER	C1033	36.909	26.139	31.703	1.00	30.12
ATOM	1576	OG	SER	C1033	36.408	25.725	30.430	1.00	30.39
ATOM	1577	N	LEU	C1034	37.291	29.100	29.905	1.00	28.42
ATOM	1578	CA	LEU	C1034	37.787	29.635	28.638	1.00	31.98
ATOM	1579	C	LEU	C1034	37.753	28.432	27.688	1.00	32.37
ATOM	1580	O	LEU	C1034	38.731	27.936	27.147	1.00	39.15
ATOM	1581	CB	LEU	C1034	39.205	30.261	28.704	1.00	29.58
ATOM	1582	CG	LEU	C1034	39.466	31.409	29.630	1.00	28.94
ATOM	1583	CD1	LEU	C1034	40.895	31.922	29.656	1.00	30.58
ATOM	1584	CD2	LEU	C1034	38.617	32.636	29.209	1.00	26.58
ATOM	1585	N	GLY	C1035	36.530	27.864	27.544	1.00	28.98
ATOM	1586	CA	GLY	C1035	36.357	26.754	26.647	1.00	24.56
ATOM	1587	C	GLY	C1035	37.171	25.481	26.790	1.00	20.81
ATOM	1588	O	GLY	C1035	37.321	24.796	25.771	1.00	21.90
ATOM	1589	N	GLY	C1036	37.326	24.968	27.997	1.00	21.82
ATOM	1590	CA	GLY	C1036	37.834	23.629	28.239	1.00	25.47

ATOM	1591	C	GLY	C1036	36.727	22.590	27.923	1.00	28.57
ATOM	1592	O	GLY	C1036	35.562	22.944	28.062	1.00	33.09
ATOM	1593	N	THR	C1037	37.098	21.424	27.446	1.00	31.18
ATOM	1594	CA	THR	C1037	36.071	20.402	27.101	1.00	31.40
ATOM	1595	C	THR	C1037	35.671	19.771	28.411	1.00	29.08
ATOM	1596	O	THR	C1037	36.402	19.322	29.267	1.00	28.43
ATOM	1597	CB	THR	C1037	36.849	19.362	26.248	1.00	35.25
ATOM	1598	OG1	THR	C1037	37.143	19.856	24.934	1.00	34.77
ATOM	1599	CG2	THR	C1037	36.056	18.071	26.103	1.00	39.81
ATOM	1600	N	PRO	C1038	34.318	19.849	28.643	1.00	28.79
ATOM	1601	CA	PRO	C1038	33.748	19.251	29.832	1.00	29.26
ATOM	1602	C	PRO	C1038	34.121	17.764	29.891	1.00	30.33
ATOM	1603	O	PRO	C1038	34.045	17.064	28.877	1.00	30.70
ATOM	1604	CB	PRO	C1038	32.262	19.472	29.632	1.00	29.45
ATOM	1605	CG	PRO	C1038	32.146	20.595	28.674	1.00	26.90
ATOM	1606	CD	PRO	C1038	33.290	20.373	27.726	1.00	26.24
ATOM	1607	N	TYR	C1039	34.507	17.239	31.019	1.00	27.10
ATOM	1608	CA	TYR	C1039	34.831	15.865	31.319	1.00	31.51
ATOM	1609	C	TYR	C1039	35.958	15.322	30.451	1.00	33.48
ATOM	1610	O	TYR	C1039	36.068	14.191	29.947	1.00	32.47
ATOM	1611	CB	TYR	C1039	33.580	14.968	31.246	1.00	29.03
ATOM	1612	CG	TYR	C1039	32.355	15.453	31.980	1.00	28.35
ATOM	1613	CD1	TYR	C1039	31.290	15.997	31.247	1.00	27.58
ATOM	1614	CD2	TYR	C1039	32.220	15.368	33.364	1.00	26.44
ATOM	1615	CE1	TYR	C1039	30.142	16.486	31.827	1.00	23.25
ATOM	1616	CE2	TYR	C1039	31.053	15.846	33.969	1.00	25.69
ATOM	1617	CZ	TYR	C1039	30.031	16.398	33.196	1.00	25.31
ATOM	1618	OH	TYR	C1039	28.870	16.776	33.851	1.00	28.82
ATOM	1619	N	CYS	C1040	36.877	16.276	30.243	1.00	37.16
ATOM	1620	CA	CYS	C1040	38.045	16.095	29.389	1.00	38.31
ATOM	1621	C	CYS	C1040	38.733	14.821	29.848	1.00	36.75
ATOM	1622	O	CYS	C1040	38.962	14.593	31.042	1.00	33.37
ATOM	1623	CB	CYS	C1040	38.886	17.360	29.511	1.00	41.12
ATOM	1624	SG	CYS	C1040	40.570	17.157	28.904	1.00	52.08
ATOM	1625	N	GLY	C1041	38.916	13.899	28.920	1.00	38.90
ATOM	1626	CA	GLY	C1041	39.550	12.613	29.230	1.00	43.75
ATOM	1627	C	GLY	C1041	38.531	11.489	29.459	1.00	46.25
ATOM	1628	O	GLY	C1041	38.940	10.313	29.384	1.00	45.71
ATOM	1629	N	MET	C1042	37.288	11.831	29.785	1.00	46.22
ATOM	1630	CA	MET	C1042	36.267	10.832	30.078	1.00	47.06
ATOM	1631	C	MET	C1042	35.471	10.388	28.874	1.00	47.05
ATOM	1632	O	MET	C1042	35.257	11.143	27.937	1.00	47.49
ATOM	1633	CB	MET	C1042	35.281	11.343	31.119	1.00	46.72
ATOM	1634	CG	MET	C1042	35.944	11.646	32.445	1.00	48.06
ATOM	1635	SD	MET	C1042	34.712	11.819	33.734	1.00	51.59
ATOM	1636	CE	MET	C1042	33.816	10.274	33.378	1.00	51.12
ATOM	1637	N	THR	C1043	35.143	9.097	28.852	1.00	48.58
ATOM	1638	CA	THR	C1043	34.359	8.548	27.745	1.00	50.37
ATOM	1639	C	THR	C1043	32.867	8.824	27.938	1.00	49.20
ATOM	1640	O	THR	C1043	32.469	8.990	29.090	1.00	48.53
ATOM	1641	CB	THR	C1043	34.541	7.022	27.715	1.00	49.50
ATOM	1642	OG1	THR	C1043	33.825	6.420	28.780	1.00	49.52
ATOM	1643	CG2	THR	C1043	36.053	6.740	27.911	1.00	48.66
ATOM	1644	N	CYS	C1044	32.090	8.784	26.869	1.00	52.39
ATOM	1645	CA	CYS	C1044	30.591	8.992	27.031	1.00	54.39
ATOM	1646	C	CYS	C1044	30.054	7.913	27.964	1.00	55.34
ATOM	1647	O	CYS	C1044	29.373	8.230	28.952	1.00	56.27

ATOM	1648	CB	CYS	C1044	29.890	9.166	25.699	1.00	54.86
ATOM	1649	SG	CYS	C1044	30.275	10.658	24.717	1.00	54.87
ATOM	1650	N	ALA	C1045	30.546	6.684	27.883	1.00	53.74
ATOM	1651	CA	ALA	C1045	30.276	5.533	28.691	1.00	53.52
ATOM	1652	C	ALA	C1045	30.319	5.704	30.200	1.00	52.95
ATOM	1653	O	ALA	C1045	29.467	5.296	31.022	1.00	52.64
ATOM	1654	CB	ALA	C1045	31.379	4.491	28.321	1.00	54.24
ATOM	1655	N	GLU	C1046	31.440	6.277	30.650	1.00	50.91
ATOM	1656	CA	GLU	C1046	31.637	6.589	32.076	1.00	48.71
ATOM	1657	C	GLU	C1046	30.675	7.673	32.539	1.00	46.60
ATOM	1658	O	GLU	C1046	30.237	7.666	33.717	1.00	44.26
ATOM	1659	CB	GLU	C1046	33.085	7.002	32.314	1.00	49.93
ATOM	1660	CG	GLU	C1046	34.115	6.109	31.628	1.00	53.13
ATOM	1661	CD	GLU	C1046	35.513	6.735	31.729	1.00	54.82
ATOM	1662	OE1	GLU	C1046	36.134	6.539	32.795	1.00	54.82
ATOM	1663	OE2	GLU	C1046	35.963	7.416	30.783	1.00	55.96
ATOM	1664	N	LEU	C1047	30.268	8.586	31.614	1.00	45.34
ATOM	1665	CA	LEU	C1047	29.331	9.632	32.066	1.00	44.07
ATOM	1666	C	LEU	C1047	27.983	9.017	32.439	1.00	42.99
ATOM	1667	O	LEU	C1047	27.530	9.215	33.576	1.00	42.01
ATOM	1668	CB	LEU	C1047	29.181	10.815	31.111	1.00	45.07
ATOM	1669	CG	LEU	C1047	30.430	11.706	30.918	1.00	44.08
ATOM	1670	CD1	LEU	C1047	30.038	12.921	30.115	1.00	45.50
ATOM	1671	CD2	LEU	C1047	31.071	12.058	32.245	1.00	42.85
ATOM	1672	N	TYR	C1048	27.409	8.182	31.588	1.00	43.22
ATOM	1673	CA	TYR	C1048	26.213	7.392	31.910	1.00	44.38
ATOM	1674	C	TYR	C1048	26.397	6.646	33.245	1.00	44.87
ATOM	1675	O	TYR	C1048	25.486	6.717	34.085	1.00	43.82
ATOM	1676	CB	TYR	C1048	25.905	6.343	30.853	1.00	44.96
ATOM	1677	CG	TYR	C1048	25.256	6.871	29.600	1.00	47.81
ATOM	1678	CD1	TYR	C1048	26.033	7.330	28.545	1.00	47.83
ATOM	1679	CD2	TYR	C1048	23.852	6.898	29.482	1.00	48.40
ATOM	1680	CE1	TYR	C1048	25.436	7.802	27.387	1.00	47.27
ATOM	1681	CE2	TYR	C1048	23.246	7.366	28.324	1.00	48.08
ATOM	1682	CZ	TYR	C1048	24.075	7.815	27.294	1.00	48.94
ATOM	1683	OH	TYR	C1048	23.413	8.274	26.168	1.00	49.94
ATOM	1684	N	GLU	C1049	27.591	6.069	33.477	1.00	42.94
ATOM	1685	CA	GLU	C1049	27.749	5.400	34.754	1.00	45.35
ATOM	1686	C	GLU	C1049	28.155	6.333	35.873	1.00	44.67
ATOM	1687	O	GLU	C1049	27.588	6.137	36.975	1.00	45.76
ATOM	1688	CB	GLU	C1049	28.683	4.171	34.686	1.00	47.30
ATOM	1689	CG	GLU	C1049	30.158	4.453	34.837	1.00	49.28
ATOM	1690	CD	GLU	C1049	31.072	3.245	35.050	1.00	50.85
ATOM	1691	OE1	GLU	C1049	31.702	2.810	34.042	1.00	51.60
ATOM	1692	OE2	GLU	C1049	31.179	2.748	36.200	1.00	49.78
ATOM	1693	N	LYS	C1050	29.038	7.320	35.685	1.00	45.45
ATOM	1694	CA	LYS	C1050	29.387	8.148	36.861	1.00	46.05
ATOM	1695	C	LYS	C1050	28.404	9.253	37.175	1.00	44.76
ATOM	1696	O	LYS	C1050	28.099	9.497	38.375	1.00	44.16
ATOM	1697	CB	LYS	C1050	30.814	8.668	36.707	1.00	49.41
ATOM	1698	CG	LYS	C1050	31.798	7.565	36.380	1.00	52.04
ATOM	1699	CD	LYS	C1050	33.285	7.938	36.456	1.00	54.77
ATOM	1700	CE	LYS	C1050	34.086	6.629	36.533	1.00	56.01
ATOM	1701	NZ	LYS	C1050	35.565	6.819	36.433	1.00	58.90
ATOM	1702	N	LEU	C1051	27.733	9.813	36.163	1.00	41.92
ATOM	1703	CA	LEU	C1051	26.746	10.866	36.552	1.00	43.18
ATOM	1704	C	LEU	C1051	25.759	10.435	37.607	1.00	43.39

FIG. 5DD

ATOM	1705	O	LEU	C1051	25.582	11.062	38.662	1.00	43.64
ATOM	1706	CB	LEU	C1051	26.145	11.496	35.307	1.00	43.49
ATOM	1707	CG	LEU	C1051	27.096	12.382	34.480	1.00	42.95
ATOM	1708	CD1	LEU	C1051	26.331	12.985	33.326	1.00	43.01
ATOM	1709	CD2	LEU	C1051	27.702	13.468	35.366	1.00	43.66
ATOM	1710	N	PRO	C1052	25.084	9.288	37.475	1.00	45.02
ATOM	1711	CA	PRO	C1052	24.140	8.817	38.470	1.00	45.84
ATOM	1712	C	PRO	C1052	24.736	8.635	39.839	1.00	47.07
ATOM	1713	O	PRO	C1052	24.088	8.826	40.880	1.00	48.20
ATOM	1714	CB	PRO	C1052	23.559	7.544	37.854	1.00	45.47
ATOM	1715	CG	PRO	C1052	23.652	7.799	36.384	1.00	44.83
ATOM	1716	CD	PRO	C1052	25.013	8.487	36.242	1.00	45.28
ATOM	1717	N	GLN	C1053	26.006	8.296	40.007	1.00	50.49
ATOM	1718	CA	GLN	C1053	26.594	8.130	41.331	1.00	52.45
ATOM	1719	C	GLN	C1053	26.921	9.462	41.976	1.00	51.74
ATOM	1720	O	GLN	C1053	27.231	9.442	43.175	1.00	51.45
ATOM	1721	CB	GLN	C1053	27.798	7.199	41.221	1.00	55.75
ATOM	1722	CG	GLN	C1053	27.411	5.794	40.768	1.00	61.04
ATOM	1723	CD	GLN	C1053	26.526	5.041	41.743	1.00	64.91
ATOM	1724	OE1	GLN	C1053	26.851	4.904	42.948	1.00	66.92
ATOM	1725	NE2	GLN	C1053	25.370	4.528	41.286	1.00	65.52
ATOM	1726	N	GLY	C1054	26.801	10.624	41.320	1.00	49.79
ATOM	1727	CA	GLY	C1054	27.061	11.874	42.052	1.00	46.62
ATOM	1728	C	GLY	C1054	28.276	12.597	41.495	1.00	44.62
ATOM	1729	O	GLY	C1054	28.683	13.662	41.920	1.00	43.65
ATOM	1730	N	TYR	C1055	28.917	12.051	40.482	1.00	45.48
ATOM	1731	CA	TYR	C1055	30.099	12.698	39.937	1.00	45.51
ATOM	1732	C	TYR	C1055	29.685	13.995	39.214	1.00	44.95
ATOM	1733	O	TYR	C1055	28.622	13.976	38.583	1.00	46.39
ATOM	1734	CB	TYR	C1055	30.767	11.776	38.932	1.00	45.73
ATOM	1735	CG	TYR	C1055	32.055	12.414	38.433	1.00	48.52
ATOM	1736	CD1	TYR	C1055	33.235	12.302	39.143	1.00	48.82
ATOM	1737	CD2	TYR	C1055	32.045	13.129	37.234	1.00	48.37
ATOM	1738	CE1	TYR	C1055	34.401	12.898	38.658	1.00	48.87
ATOM	1739	CE2	TYR	C1055	33.178	13.723	36.737	1.00	47.42
ATOM	1740	CZ	TYR	C1055	34.354	13.582	37.459	1.00	49.27
ATOM	1741	OH	TYR	C1055	35.488	14.170	36.952	1.00	48.77
ATOM	1742	N	ARG	C1056	30.485	15.051	39.252	1.00	40.28
ATOM	1743	CA	ARG	C1056	30.189	16.276	38.566	1.00	38.71
ATOM	1744	C	ARG	C1056	31.481	17.012	38.176	1.00	39.85
ATOM	1745	O	ARG	C1056	32.472	16.797	38.879	1.00	42.11
ATOM	1746	CB	ARG	C1056	29.407	17.281	39.408	1.00	38.04
ATOM	1747	CG	ARG	C1056	27.996	17.004	39.890	1.00	37.78
ATOM	1748	CD	ARG	C1056	27.022	16.584	38.810	1.00	34.37
ATOM	1749	NE	ARG	C1056	25.677	16.380	39.370	1.00	32.75
ATOM	1750	CZ	ARG	C1056	25.172	15.135	39.461	1.00	34.13
ATOM	1751	NH1	ARG	C1056	23.934	15.014	39.951	1.00	33.89
ATOM	1752	NH2	ARG	C1056	25.884	14.083	39.063	1.00	31.70
ATOM	1753	N	LEU	C1057	31.450	17.843	37.130	1.00	37.74
ATOM	1754	CA	LEU	C1057	32.615	18.640	36.829	1.00	38.61
ATOM	1755	C	LEU	C1057	33.280	19.260	38.062	1.00	37.18
ATOM	1756	O	LEU	C1057	32.759	19.829	39.007	1.00	36.18
ATOM	1757	CB	LEU	C1057	32.223	19.785	35.886	1.00	39.58
ATOM	1758	CG	LEU	C1057	31.870	19.236	34.492	1.00	40.26
ATOM	1759	CD1	LEU	C1057	31.190	20.384	33.790	1.00	41.53
ATOM	1760	CD2	LEU	C1057	33.089	18.719	33.746	1.00	40.04
ATOM	1761	N	GLU	C1058	34.597	19.231	37.962	1.00	38.47

FIG. 5EE

ATOM	1762	CA	GLU	C1058	35.494	19.715	39.003	1.00	40.99
ATOM	1763	C	GLU	C1058	35.655	21.237	38.941	1.00	37.60
ATOM	1764	O	GLU	C1058	35.665	21.759	37.841	1.00	37.18
ATOM	1765	CB	GLU	C1058	36.808	18.952	38.778	1.00	43.93
ATOM	1766	CG	GLU	C1058	37.256	18.728	37.367	1.00	49.34
ATOM	1767	CD	GLU	C1058	36.540	18.005	36.265	1.00	51.18
ATOM	1768	OE1	GLU	C1058	36.581	18.538	35.121	1.00	50.19
ATOM	1769	OE2	GLU	C1058	35.931	16.902	36.361	1.00	52.82
ATOM	1770	N	LYS	C1059	35.708	21.975	40.005	1.00	35.88
ATOM	1771	CA	LYS	C1059	35.948	23.424	39.950	1.00	40.12
ATOM	1772	C	LYS	C1059	37.345	23.831	39.473	1.00	41.54
ATOM	1773	O	LYS	C1059	38.332	23.431	40.095	1.00	41.88
ATOM	1774	CB	LYS	C1059	35.946	23.896	41.417	1.00	39.21
ATOM	1775	CG	LYS	C1059	35.984	25.413	41.569	1.00	41.97
ATOM	1776	CD	LYS	C1059	35.953	25.810	43.048	1.00	43.62
ATOM	1777	CE	LYS	C1059	37.349	25.786	43.641	1.00	43.92
ATOM	1778	NZ	LYS	C1059	38.192	26.906	43.099	1.00	44.39
ATOM	1779	N	PRO	C1060	37.498	24.651	38.439	1.00	41.99
ATOM	1780	CA	PRO	C1060	38.795	25.166	38.040	1.00	42.27
ATOM	1781	C	PRO	C1060	39.441	25.920	39.186	1.00	42.45
ATOM	1782	O	PRO	C1060	38.840	26.618	39.996	1.00	40.76
ATOM	1783	CB	PRO	C1060	38.529	26.115	36.894	1.00	43.06
ATOM	1784	CG	PRO	C1060	37.145	25.765	36.416	1.00	41.60
ATOM	1785	CD	PRO	C1060	36.408	25.170	37.589	1.00	41.74
ATOM	1786	N	LEU	C1061	40.773	25.843	39.287	1.00	44.11
ATOM	1787	CA	LEU	C1061	41.557	26.440	40.325	1.00	44.84
ATOM	1788	C	LEU	C1061	41.416	27.941	40.443	1.00	44.71
ATOM	1789	O	LEU	C1061	41.441	28.470	41.567	1.00	45.26
ATOM	1790	CB	LEU	C1061	43.036	26.089	40.055	1.00	48.79
ATOM	1791	CG	LEU	C1061	43.314	24.624	40.459	1.00	52.11
ATOM	1792	CD1	LEU	C1061	44.673	24.204	39.897	1.00	53.08
ATOM	1793	CD2	LEU	C1061	43.288	24.512	41.984	1.00	52.05
ATOM	1794	N	ASN	C1062	41.247	28.623	39.321	1.00	44.44
ATOM	1795	CA	ASN	C1062	41.112	30.085	39.327	1.00	44.45
ATOM	1796	C	ASN	C1062	39.661	30.582	39.363	1.00	44.24
ATOM	1797	O	ASN	C1062	39.394	31.757	39.073	1.00	42.70
ATOM	1798	CB	ASN	C1062	41.811	30.536	38.059	1.00	47.14
ATOM	1799	CG	ASN	C1062	41.018	30.280	36.799	1.00	50.71
ATOM	1800	OD1	ASN	C1062	40.297	29.260	36.680	1.00	55.26
ATOM	1801	ND2	ASN	C1062	41.160	31.208	35.873	1.00	49.84
ATOM	1802	N	CYS	C1063	38.727	29.727	39.787	1.00	40.21
ATOM	1803	CA	CYS	C1063	37.312	30.006	39.917	1.00	39.16
ATOM	1804	C	CYS	C1063	36.922	30.226	41.375	1.00	40.26
ATOM	1805	O	CYS	C1063	37.149	29.298	42.177	1.00	38.11
ATOM	1806	CB	CYS	C1063	36.476	28.796	39.430	1.00	36.02
ATOM	1807	SG	CYS	C1063	34.684	29.162	39.283	1.00	36.25
ATOM	1808	N	ASP	C1064	36.179	31.287	41.675	1.00	39.98
ATOM	1809	CA	ASP	C1064	35.704	31.514	43.034	1.00	42.23
ATOM	1810	C	ASP	C1064	34.623	30.474	43.367	1.00	43.63
ATOM	1811	O	ASP	C1064	33.885	29.998	42.516	1.00	42.13
ATOM	1812	CB	ASP	C1064	35.166	32.915	43.277	1.00	44.24
ATOM	1813	CG	ASP	C1064	34.744	33.348	44.660	1.00	47.38
ATOM	1814	OD1	ASP	C1064	35.591	34.016	45.335	1.00	49.14
ATOM	1815	OD2	ASP	C1064	33.594	33.165	45.169	1.00	46.30
ATOM	1816	N	ASP	C1065	34.571	30.128	44.646	1.00	44.20
ATOM	1817	CA	ASP	C1065	33.681	29.213	45.285	1.00	46.41
ATOM	1818	C	ASP	C1065	32.214	29.629	45.059	1.00	46.09

FIG. 5FF

ATOM	1819	O	ASP	C1065	31.383	28.772	44.807	1.00	45.90
ATOM	1820	CB	ASP	C1065	33.999	29.111	46.780	1.00	49.84
ATOM	1821	CG	ASP	C1065	34.972	28.020	47.179	1.00	54.04
ATOM	1822	OD1	ASP	C1065	35.370	27.139	46.384	1.00	54.54
ATOM	1823	OD2	ASP	C1065	35.412	27.941	48.364	1.00	56.55
ATOM	1824	N	GLU	C1066	31.932	30.931	44.991	1.00	46.33
ATOM	1825	CA	GLU	C1066	30.585	31.364	44.699	1.00	46.37
ATOM	1826	C	GLU	C1066	30.162	30.946	43.279	1.00	43.58
ATOM	1827	O	GLU	C1066	28.974	30.622	43.161	1.00	40.53
ATOM	1828	CB	GLU	C1066	30.362	32.870	44.901	1.00	47.78
ATOM	1829	CG	GLU	C1066	30.464	33.371	46.327	1.00	51.27
ATOM	1830	CD	GLU	C1066	30.147	34.853	46.483	1.00	54.46
ATOM	1831	OE1	GLU	C1066	30.977	35.632	47.023	1.00	56.49
ATOM	1832	OE2	GLU	C1066	29.039	35.278	46.075	1.00	54.91
ATOM	1833	N	VAL	C1067	31.031	31.026	42.267	1.00	40.02
ATOM	1834	CA	VAL	C1067	30.592	30.670	40.914	1.00	38.39
ATOM	1835	C	VAL	C1067	30.361	29.166	40.750	1.00	38.56
ATOM	1836	O	VAL	C1067	29.492	28.741	39.975	1.00	35.01
ATOM	1837	CB	VAL	C1067	31.561	31.094	39.797	1.00	37.83
ATOM	1838	CG1	VAL	C1067	31.071	30.760	38.416	1.00	34.84
ATOM	1839	CG2	VAL	C1067	31.809	32.609	39.878	1.00	39.35
ATOM	1840	N	TYR	C1068	31.258	28.419	41.393	1.00	37.89
ATOM	1841	CA	TYR	C1068	31.203	26.969	41.346	1.00	38.97
ATOM	1842	C	TYR	C1068	29.924	26.510	42.044	1.00	40.70
ATOM	1843	O	TYR	C1068	29.265	25.613	41.492	1.00	38.63
ATOM	1844	CB	TYR	C1068	32.437	26.278	41.913	1.00	37.20
ATOM	1845	CG	TYR	C1068	32.470	24.770	41.798	1.00	35.05
ATOM	1846	CD1	TYR	C1068	32.535	24.158	40.556	1.00	34.59
ATOM	1847	CD2	TYR	C1068	32.431	23.934	42.903	1.00	35.51
ATOM	1848	CE1	TYR	C1068	32.536	22.785	40.405	1.00	33.51
ATOM	1849	CE2	TYR	C1068	32.456	22.549	42.800	1.00	33.38
ATOM	1850	CZ	TYR	C1068	32.540	22.006	41.540	1.00	33.70
ATOM	1851	OH	TYR	C1068	32.545	20.637	41.342	1.00	37.05
ATOM	1852	N	ASP	C1069	29.573	27.177	43.159	1.00	42.06
ATOM	1853	CA	ASP	C1069	28.316	26.862	43.806	1.00	42.68
ATOM	1854	C	ASP	C1069	27.124	27.069	42.869	1.00	40.99
ATOM	1855	O	ASP	C1069	26.233	26.193	42.884	1.00	40.08
ATOM	1856	CB	ASP	C1069	28.116	27.676	45.094	1.00	47.98
ATOM	1857	CG	ASP	C1069	28.983	27.092	46.212	1.00	53.70
ATOM	1858	OD1	ASP	C1069	29.487	25.940	46.045	1.00	55.80
ATOM	1859	OD2	ASP	C1069	29.161	27.786	47.254	1.00	55.99
ATOM	1860	N	LEU	C1070	27.080	28.150	42.087	1.00	36.81
ATOM	1861	CA	LEU	C1070	25.977	28.308	41.140	1.00	36.03
ATOM	1862	C	LEU	C1070	25.905	27.172	40.123	1.00	34.83
ATOM	1863	O	LEU	C1070	24.833	26.703	39.743	1.00	32.57
ATOM	1864	CB	LEU	C1070	26.131	29.666	40.472	1.00	33.68
ATOM	1865	CG	LEU	C1070	25.095	30.113	39.458	1.00	35.12
ATOM	1866	CD1	LEU	C1070	23.674	29.955	40.003	1.00	34.71
ATOM	1867	CD2	LEU	C1070	25.391	31.582	39.084	1.00	34.63
ATOM	1868	N	MET	C1071	27.036	26.703	39.602	1.00	36.71
ATOM	1869	CA	MET	C1071	27.131	25.568	38.706	1.00	37.17
ATOM	1870	C	MET	C1071	26.555	24.302	39.372	1.00	36.93
ATOM	1871	O	MET	C1071	25.808	23.574	38.735	1.00	36.82
ATOM	1872	CB	MET	C1071	28.569	25.145	38.294	1.00	35.35
ATOM	1873	CG	MET	C1071	29.354	26.145	37.465	1.00	35.64
ATOM	1874	SD	MET	C1071	31.096	25.645	37.207	1.00	32.11
ATOM	1875	CE	MET	C1071	31.839	27.209	36.753	1.00	34.27

FIG. 5GG

ATOM	1876	N	ARG	C1072	26.959	23.943	40.580	1.00	36.71
ATOM	1877	CA	ARG	C1072	26.550	22.771	41.323	1.00	37.27
ATOM	1878	C	ARG	C1072	25.039	22.687	41.557	1.00	36.15
ATOM	1879	O	ARG	C1072	24.384	21.638	41.587	1.00	37.31
ATOM	1880	CB	ARG	C1072	27.272	22.810	42.713	1.00	39.01
ATOM	1881	CG	ARG	C1072	28.773	22.514	42.664	1.00	38.84
ATOM	1882	CD	ARG	C1072	29.110	21.260	41.887	1.00	40.99
ATOM	1883	NE	ARG	C1072	28.618	20.088	42.608	1.00	45.98
ATOM	1884	CZ	ARG	C1072	29.217	19.090	43.239	1.00	46.52
ATOM	1885	NH1	ARG	C1072	30.532	18.968	43.255	1.00	44.60
ATOM	1886	NH2	ARG	C1072	28.428	18.173	43.842	1.00	46.54
ATOM	1887	N	GLN	C1073	24.427	23.832	41.775	1.00	36.36
ATOM	1888	CA	GLN	C1073	22.986	24.010	41.934	1.00	36.84
ATOM	1889	C	GLN	C1073	22.289	23.680	40.612	1.00	35.17
ATOM	1890	O	GLN	C1073	21.240	23.043	40.616	1.00	36.12
ATOM	1891	CB	GLN	C1073	22.690	25.436	42.324	1.00	40.62
ATOM	1892	CG	GLN	C1073	22.926	25.928	43.737	1.00	44.26
ATOM	1893	CD	GLN	C1073	22.601	27.425	43.797	1.00	48.97
ATOM	1894	OE1	GLN	C1073	22.895	28.160	44.746	1.00	50.88
ATOM	1895	NE2	GLN	C1073	21.954	27.977	42.770	1.00	50.58
ATOM	1896	N	CYS	C1074	22.888	23.925	39.463	1.00	34.02
ATOM	1897	CA	CYS	C1074	22.346	23.554	38.175	1.00	33.44
ATOM	1898	C	CYS	C1074	22.300	22.048	37.953	1.00	32.85
ATOM	1899	O	CYS	C1074	21.595	21.573	37.050	1.00	28.15
ATOM	1900	CB	CYS	C1074	23.165	24.222	37.052	1.00	32.80
ATOM	1901	SG	CYS	C1074	22.926	26.054	36.945	1.00	29.54
ATOM	1902	N	TRP	C1075	23.155	21.300	38.651	1.00	34.38
ATOM	1903	CA	TRP	C1075	23.323	19.869	38.394	1.00	36.36
ATOM	1904	C	TRP	C1075	22.772	19.008	39.538	1.00	37.35
ATOM	1905	O	TRP	C1075	23.378	17.961	39.809	1.00	36.14
ATOM	1906	CB	TRP	C1075	24.797	19.516	38.184	1.00	31.61
ATOM	1907	CG	TRP	C1075	25.554	20.319	37.170	1.00	32.01
ATOM	1908	CD1	TRP	C1075	25.035	20.735	35.945	1.00	30.72
ATOM	1909	CD2	TRP	C1075	26.905	20.792	37.215	1.00	27.71
ATOM	1910	NE1	TRP	C1075	26.028	21.458	35.263	1.00	27.75
ATOM	1911	CE2	TRP	C1075	27.165	21.473	36.015	1.00	27.79
ATOM	1912	CE3	TRP	C1075	27.923	20.731	38.161	1.00	29.11
ATOM	1913	CZ2	TRP	C1075	28.393	22.095	35.707	1.00	27.12
ATOM	1914	CZ3	TRP	C1075	29.172	21.338	37.861	1.00	27.92
ATOM	1915	CH2	TRP	C1075	29.394	22.010	36.640	1.00	26.04
ATOM	1916	N	ARG	C1076	21.729	19.503	40.206	1.00	38.82
ATOM	1917	CA	ARG	C1076	21.190	18.763	41.348	1.00	40.61
ATOM	1918	C	ARG	C1076	20.509	17.546	40.743	1.00	40.05
ATOM	1919	O	ARG	C1076	19.967	17.688	39.634	1.00	40.43
ATOM	1920	CB	ARG	C1076	20.272	19.608	42.208	1.00	42.35
ATOM	1921	CG	ARG	C1076	20.932	20.378	43.334	1.00	45.64
ATOM	1922	CD	ARG	C1076	20.106	21.505	43.893	1.00	49.70
ATOM	1923	NE	ARG	C1076	20.769	22.441	44.800	1.00	52.00
ATOM	1924	CZ	ARG	C1076	20.478	23.723	45.050	1.00	51.66
ATOM	1925	NH1	ARG	C1076	19.508	24.410	44.455	1.00	50.03
ATOM	1926	NH2	ARG	C1076	21.238	24.353	45.949	1.00	52.86
ATOM	1927	N	GLU	C1077	20.598	16.392	41.374	1.00	41.20
ATOM	1928	CA	GLU	C1077	19.944	15.200	40.818	1.00	42.65
ATOM	1929	C	GLU	C1077	18.447	15.393	40.555	1.00	38.60
ATOM	1930	O	GLU	C1077	17.929	15.043	39.481	1.00	35.94
ATOM	1931	CB	GLU	C1077	20.198	13.968	41.695	1.00	45.87
ATOM	1932	CG	GLU	C1077	20.013	12.643	40.962	1.00	50.08

FIG. 5HH

ATOM	1933	CD	GLU	C1077	20.183	11.401	41.819	1.00	54.47
ATOM	1934	OE1	GLU	C1077	20.561	10.312	41.308	1.00	57.69
ATOM	1935	OE2	GLU	C1077	19.955	11.404	43.055	1.00	56.30
ATOM	1936	N	LYS	C1078	17.706	15.887	41.503	1.00	39.48
ATOM	1937	CA	LYS	C1078	16.243	16.090	41.262	1.00	40.94
ATOM	1938	C	LYS	C1078	16.079	17.369	40.455	1.00	40.21
ATOM	1939	O	LYS	C1078	16.480	18.449	40.854	1.00	38.01
ATOM	1940	CB	LYS	C1078	15.475	16.240	42.568	1.00	43.70
ATOM	1941	CG	LYS	C1078	15.829	15.188	43.605	1.00	46.67
ATOM	1942	CD	LYS	C1078	15.384	15.538	45.015	1.00	49.04
ATOM	1943	CE	LYS	C1078	15.414	14.237	45.826	1.00	53.53
ATOM	1944	NZ	LYS	C1078	14.894	14.422	47.213	1.00	55.30
ATOM	1945	N	PRO	C1079	15.476	17.282	39.288	1.00	38.88
ATOM	1946	CA	PRO	C1079	15.298	18.465	38.451	1.00	39.64
ATOM	1947	C	PRO	C1079	14.654	19.621	39.182	1.00	40.23
ATOM	1948	O	PRO	C1079	15.091	20.778	39.078	1.00	39.41
ATOM	1949	CB	PRO	C1079	14.521	17.924	37.259	1.00	36.96
ATOM	1950	CG	PRO	C1079	14.929	16.461	37.199	1.00	35.65
ATOM	1951	CD	PRO	C1079	14.988	16.035	38.647	1.00	36.92
ATOM	1952	N	TYR	C1080	13.657	19.387	40.028	1.00	41.92
ATOM	1953	CA	TYR	C1080	12.882	20.406	40.717	1.00	43.85
ATOM	1954	C	TYR	C1080	13.587	21.140	41.824	1.00	43.51
ATOM	1955	O	TYR	C1080	13.109	22.140	42.388	1.00	43.12
ATOM	1956	CB	TYR	C1080	11.505	19.831	41.176	1.00	45.60
ATOM	1957	CG	TYR	C1080	11.697	18.722	42.194	1.00	47.84
ATOM	1958	CD1	TYR	C1080	11.973	18.993	43.531	1.00	49.35
ATOM	1959	CD2	TYR	C1080	11.636	17.389	41.798	1.00	49.13
ATOM	1960	CE1	TYR	C1080	12.146	17.958	44.445	1.00	50.14
ATOM	1961	CE2	TYR	C1080	11.806	16.370	42.704	1.00	50.24
ATOM	1962	CZ	TYR	C1080	12.058	16.656	44.030	1.00	50.60
ATOM	1963	OH	TYR	C1080	12.242	15.597	44.908	1.00	53.21
ATOM	1964	N	GLU	C1081	14.799	20.700	42.144	1.00	44.60
ATOM	1965	CA	GLU	C1081	15.638	21.420	43.102	1.00	44.07
ATOM	1966	C	GLU	C1081	16.559	22.432	42.419	1.00	40.19
ATOM	1967	O	GLU	C1081	17.250	23.137	43.126	1.00	37.60
ATOM	1968	CB	GLU	C1081	16.508	20.467	43.922	1.00	45.52
ATOM	1969	CG	GLU	C1081	15.648	19.808	45.014	1.00	50.79
ATOM	1970	CD	GLU	C1081	16.627	18.944	45.789	1.00	54.16
ATOM	1971	OE1	GLU	C1081	16.879	19.248	46.968	1.00	58.46
ATOM	1972	OE2	GLU	C1081	17.210	17.991	45.250	1.00	55.69
ATOM	1973	N	ARG	C1082	16.647	22.458	41.105	1.00	39.28
ATOM	1974	CA	ARG	C1082	17.497	23.363	40.367	1.00	37.58
ATOM	1975	C	ARG	C1082	16.828	24.740	40.394	1.00	38.63
ATOM	1976	O	ARG	C1082	15.612	24.910	40.383	1.00	40.38
ATOM	1977	CB	ARG	C1082	17.704	22.926	38.895	1.00	36.08
ATOM	1978	CG	ARG	C1082	18.469	21.599	38.779	1.00	36.20
ATOM	1979	CD	ARG	C1082	18.609	20.955	37.417	1.00	33.59
ATOM	1980	NE	ARG	C1082	18.832	19.501	37.535	1.00	34.00
ATOM	1981	CZ	ARG	C1082	18.469	18.515	36.714	1.00	32.08
ATOM	1982	NH1	ARG	C1082	17.822	18.762	35.569	1.00	31.72
ATOM	1983	NH2	ARG	C1082	18.708	17.204	36.908	1.00	31.86
ATOM	1984	N	PRO	C1083	17.667	25.772	40.289	1.00	34.94
ATOM	1985	CA	PRO	C1083	17.201	27.135	40.253	1.00	32.78
ATOM	1986	C	PRO	C1083	16.556	27.432	38.912	1.00	33.70
ATOM	1987	O	PRO	C1083	16.641	26.652	37.947	1.00	31.92
ATOM	1988	CB	PRO	C1083	18.446	28.006	40.398	1.00	27.76
ATOM	1989	CG	PRO	C1083	19.621	27.077	40.186	1.00	30.28

FIG. 5II

ATOM	1990	CD	PRO	C1083	19.139	25.661	40.404	1.00	32.35
ATOM	1991	N	SER	C1084	15.816	28.558	38.933	1.00	31.68
ATOM	1992	CA	SER	C1084	15.199	29.032	37.705	1.00	31.93
ATOM	1993	C	SER	C1084	16.210	30.014	37.080	1.00	31.48
ATOM	1994	O	SER	C1084	17.144	30.514	37.733	1.00	29.39
ATOM	1995	CB	SER	C1084	13.873	29.704	38.085	1.00	31.83
ATOM	1996	OG	SER	C1084	14.132	31.022	38.595	1.00	32.90
ATOM	1997	N	PHE	C1085	16.099	30.275	35.783	1.00	30.49
ATOM	1998	CA	PHE	C1085	16.882	31.203	35.046	1.00	31.87
ATOM	1999	C	PHE	C1085	16.731	32.620	35.612	1.00	35.04
ATOM	2000	O	PHE	C1085	17.778	33.269	35.568	1.00	34.20
ATOM	2001	CB	PHE	C1085	16.631	31.270	33.533	1.00	29.72
ATOM	2002	CG	PHE	C1085	17.113	30.035	32.829	1.00	29.58
ATOM	2003	CD1	PHE	C1085	16.278	29.113	32.259	1.00	27.05
ATOM	2004	CD2	PHE	C1085	18.513	29.847	32.765	1.00	28.92
ATOM	2005	CE1	PHE	C1085	16.764	28.002	31.606	1.00	29.03
ATOM	2006	CE2	PHE	C1085	18.999	28.739	32.078	1.00	31.04
ATOM	2007	CZ	PHE	C1085	18.172	27.810	31.537	1.00	29.42
ATOM	2008	N	ALA	C1086	15.538	32.967	36.152	1.00	34.52
ATOM	2009	CA	ALA	C1086	15.461	34.251	36.811	1.00	36.36
ATOM	2010	C	ALA	C1086	16.330	34.297	38.053	1.00	35.05
ATOM	2011	O	ALA	C1086	16.940	35.370	38.305	1.00	33.03
ATOM	2012	CB	ALA	C1086	13.991	34.579	37.178	1.00	36.02
ATOM	2013	N	GLN	C1087	16.403	33.210	38.808	1.00	34.48
ATOM	2014	CA	GLN	C1087	17.187	33.187	40.043	1.00	37.34
ATOM	2015	C	GLN	C1087	18.692	33.172	39.718	1.00	36.23
ATOM	2016	O	GLN	C1087	19.488	33.831	40.397	1.00	34.12
ATOM	2017	CB	GLN	C1087	16.898	31.991	40.963	1.00	39.18
ATOM	2018	CG	GLN	C1087	15.465	31.766	41.372	1.00	41.60
ATOM	2019	CD	GLN	C1087	15.181	30.507	42.185	1.00	41.95
ATOM	2020	OE1	GLN	C1087	14.644	30.647	43.307	1.00	43.26
ATOM	2021	NE2	GLN	C1087	15.463	29.299	41.755	1.00	38.28
ATOM	2022	N	ILE	C1088	19.023	32.489	38.609	1.00	36.91
ATOM	2023	CA	ILE	C1088	20.421	32.470	38.143	1.00	34.98
ATOM	2024	C	ILE	C1088	20.850	33.891	37.730	1.00	36.64
ATOM	2025	O	ILE	C1088	21.994	34.310	37.999	1.00	38.60
ATOM	2026	CB	ILE	C1088	20.707	31.497	37.017	1.00	31.65
ATOM	2027	CG1	ILE	C1088	20.729	30.014	37.479	1.00	28.80
ATOM	2028	CG2	ILE	C1088	22.108	31.715	36.417	1.00	32.45
ATOM	2029	CD1	ILE	C1088	20.354	29.149	36.296	1.00	24.89
ATOM	2030	N	LEU	C1089	20.006	34.626	37.037	1.00	36.93
ATOM	2031	CA	LEU	C1089	20.288	36.010	36.641	1.00	38.78
ATOM	2032	C	LEU	C1089	20.504	36.934	37.835	1.00	39.65
ATOM	2033	O	LEU	C1089	21.396	37.812	37.840	1.00	38.19
ATOM	2034	CB	LEU	C1089	19.192	36.562	35.727	1.00	39.78
ATOM	2035	CG	LEU	C1089	19.421	37.938	35.087	1.00	41.64
ATOM	2036	CD1	LEU	C1089	20.497	37.892	34.014	1.00	39.98
ATOM	2037	CD2	LEU	C1089	18.113	38.470	34.492	1.00	40.00
ATOM	2038	N	VAL	C1090	19.730	36.740	38.902	1.00	41.42
ATOM	2039	CA	VAL	C1090	19.894	37.611	40.075	1.00	43.28
ATOM	2040	C	VAL	C1090	21.247	37.342	40.727	1.00	43.77
ATOM	2041	O	VAL	C1090	21.948	38.289	41.115	1.00	45.25
ATOM	2042	CB	VAL	C1090	18.759	37.424	41.081	1.00	44.41
ATOM	2043	CG1	VAL	C1090	19.139	38.123	42.387	1.00	45.32
ATOM	2044	CG2	VAL	C1090	17.422	37.989	40.595	1.00	45.38
ATOM	2045	N	SER	C1091	21.634	36.074	40.924	1.00	43.36
ATOM	2046	CA	SER	C1091	22.921	35.817	41.543	1.00	45.59

ATOM	2047	C	SER	C1091	24.044	36.357	40.663	1.00	43.29
ATOM	2048	O	SER	C1091	24.987	36.921	41.231	1.00	43.04
ATOM	2049	CB	SER	C1091	23.056	34.332	41.946	1.00	48.54
ATOM	2050	OG	SER	C1091	22.563	33.588	40.846	1.00	54.84
ATOM	2051	N	LEU	C1092	23.971	36.337	39.335	1.00	38.97
ATOM	2052	CA	LEU	C1092	25.098	36.849	38.570	1.00	37.84
ATOM	2053	C	LEU	C1092	25.118	38.383	38.604	1.00	39.82
ATOM	2054	O	LEU	C1092	26.207	38.957	38.627	1.00	35.95
ATOM	2055	CB	LEU	C1092	25.098	36.309	37.150	1.00	35.04
ATOM	2056	CG	LEU	C1092	25.301	34.789	36.982	1.00	33.88
ATOM	2057	CD1	LEU	C1092	24.655	34.383	35.662	1.00	33.07
ATOM	2058	CD2	LEU	C1092	26.773	34.446	37.016	1.00	34.04
ATOM	2059	N	ASN	C1093	23.942	39.039	38.597	1.00	41.48
ATOM	2060	CA	ASN	C1093	23.920	40.525	38.641	1.00	43.61
ATOM	2061	C	ASN	C1093	24.527	41.074	39.936	1.00	44.92
ATOM	2062	O	ASN	C1093	25.166	42.135	39.946	1.00	44.64
ATOM	2063	CB	ASN	C1093	22.509	41.084	38.434	1.00	42.95
ATOM	2064	CG	ASN	C1093	21.996	41.095	37.021	1.00	44.32
ATOM	2065	OD1	ASN	C1093	20.771	41.140	36.726	1.00	46.00
ATOM	2066	ND2	ASN	C1093	22.859	41.098	36.023	1.00	43.94
ATOM	2067	N	ARG	C1094	24.374	40.336	41.043	1.00	46.27
ATOM	2068	CA	ARG	C1094	24.957	40.724	42.334	1.00	47.34
ATOM	2069	C	ARG	C1094	26.473	40.529	42.302	1.00	47.18
ATOM	2070	O	ARG	C1094	27.308	41.386	42.683	1.00	48.73
ATOM	2071	CB	ARG	C1094	24.207	39.952	43.397	1.00	48.52
ATOM	2072	CG	ARG	C1094	24.600	40.135	44.831	1.00	53.04
ATOM	2073	CD	ARG	C1094	25.893	39.506	45.266	1.00	55.51
ATOM	2074	NE	ARG	C1094	25.811	38.266	46.057	1.00	58.34
ATOM	2075	CZ	ARG	C1094	26.945	37.595	46.345	1.00	58.94
ATOM	2076	NH1	ARG	C1094	28.144	37.993	45.942	1.00	58.67
ATOM	2077	NH2	ARG	C1094	26.892	36.486	47.071	1.00	60.47
ATOM	2078	N	MET	C1095	26.945	39.465	41.654	1.00	43.61
ATOM	2079	CA	MET	C1095	28.378	39.288	41.439	1.00	41.53
ATOM	2080	C	MET	C1095	28.854	40.419	40.535	1.00	37.96
ATOM	2081	O	MET	C1095	29.993	40.855	40.670	1.00	39.00
ATOM	2082	CB	MET	C1095	28.772	37.969	40.755	1.00	39.83
ATOM	2083	CG	MET	C1095	28.636	36.767	41.644	1.00	42.24
ATOM	2084	SD	MET	C1095	28.588	35.160	40.819	1.00	43.52
ATOM	2085	CE	MET	C1095	29.492	34.284	42.084	1.00	43.64
ATOM	2086	N	LEU	C1096	28.128	40.770	39.489	1.00	38.63
ATOM	2087	CA	LEU	C1096	28.592	41.811	38.583	1.00	40.32
ATOM	2088	C	LEU	C1096	28.726	43.159	39.300	1.00	45.56
ATOM	2089	O	LEU	C1096	29.676	43.913	39.027	1.00	43.98
ATOM	2090	CB	LEU	C1096	27.705	41.881	37.363	1.00	38.78
ATOM	2091	CG	LEU	C1096	27.859	40.853	36.254	1.00	36.87
ATOM	2092	CD1	LEU	C1096	26.623	40.917	35.364	1.00	37.20
ATOM	2093	CD2	LEU	C1096	29.157	41.041	35.484	1.00	36.07
ATOM	2094	N	GLU	C1097	27.840	43.531	40.207	1.00	50.71
ATOM	2095	CA	GLU	C1097	27.911	44.809	40.888	1.00	56.21
ATOM	2096	C	GLU	C1097	28.997	45.073	41.913	1.00	57.95
ATOM	2097	O	GLU	C1097	29.115	46.249	42.308	1.00	58.28
ATOM	2098	CB	GLU	C1097	26.511	45.083	41.496	1.00	59.17
ATOM	2099	CG	GLU	C1097	25.588	45.556	40.362	1.00	62.97
ATOM	2100	CD	GLU	C1097	25.880	46.999	39.984	1.00	65.89
ATOM	2101	OE1	GLU	C1097	26.772	47.604	40.633	1.00	67.34
ATOM	2102	OE2	GLU	C1097	25.159	47.465	39.064	1.00	68.13
ATOM	2103	N	GLU	C1098	29.832	44.134	42.340	1.00	59.64

FIG. 5KK

ATOM	2104	CA	GLU	C1098	30.923	44.413	43.251	1.00	62.30
ATOM	2105	C	GLU	C1098	32.317	44.135	42.709	1.00	61.47
ATOM	2106	O	GLU	C1098	32.699	43.098	42.165	1.00	63.11
ATOM	2107	CB	GLU	C1098	30.721	43.618	44.546	1.00	63.71
ATOM	2108	CG	GLU	C1098	30.447	42.141	44.289	1.00	64.85
ATOM	2109	CD	GLU	C1098	30.147	41.457	45.616	1.00	66.52
ATOM	2110	OE1	GLU	C1098	29.135	41.807	46.262	1.00	67.90
ATOM	2111	OE2	GLU	C1098	30.943	40.587	46.021	1.00	67.37
ATOM	2112	N	ARG	C1099	33.234	45.047	43.011	1.00	62.10
ATOM	2113	CA	ARG	C1099	34.637	45.044	42.675	1.00	60.00
ATOM	2114	C	ARG	C1099	35.404	43.736	42.782	1.00	58.76
ATOM	2115	O	ARG	C1099	36.433	43.655	42.072	1.00	60.07
ATOM	2116	CB	ARG	C1099	35.327	46.048	43.623	1.00	61.21
ATOM	2117	N	LYS	C1100	35.024	42.747	43.594	1.00	56.32
ATOM	2118	CA	LYS	C1100	35.843	41.536	43.624	1.00	55.34
ATOM	2119	C	LYS	C1100	35.881	40.863	42.258	1.00	53.59
ATOM	2120	O	LYS	C1100	35.083	41.060	41.366	1.00	53.08
ATOM	2121	CB	LYS	C1100	35.416	40.629	44.760	1.00	56.50
ATOM	2122	CG	LYS	C1100	34.580	39.418	44.451	1.00	57.25
ATOM	2123	CD	LYS	C1100	33.972	38.745	45.669	1.00	57.47
ATOM	2124	CE	LYS	C1100	34.923	37.780	46.342	1.00	59.43
ATOM	2125	NZ	LYS	C1100	34.265	36.502	46.768	1.00	59.87
ATOM	2126	N	THR	C1101	36.911	40.037	42.055	1.00	53.38
ATOM	2127	CA	THR	C1101	37.201	39.285	40.840	1.00	48.64
ATOM	2128	C	THR	C1101	36.746	37.835	41.057	1.00	46.24
ATOM	2129	O	THR	C1101	37.229	37.252	42.047	1.00	45.91
ATOM	2130	CB	THR	C1101	38.694	39.327	40.489	1.00	47.56
ATOM	2131	OG1	THR	C1101	39.019	40.606	39.939	1.00	46.44
ATOM	2132	CG2	THR	C1101	39.094	38.266	39.469	1.00	45.84
ATOM	2133	N	TYR	C1102	35.884	37.335	40.167	1.00	41.77
ATOM	2134	CA	TYR	C1102	35.366	35.978	40.426	1.00	40.39
ATOM	2135	C	TYR	C1102	36.129	34.910	39.691	1.00	40.66
ATOM	2136	O	TYR	C1102	36.056	33.736	40.095	1.00	42.76
ATOM	2137	CB	TYR	C1102	33.858	35.910	40.100	1.00	38.06
ATOM	2138	CG	TYR	C1102	33.074	36.622	41.174	1.00	39.42
ATOM	2139	CD1	TYR	C1102	32.812	37.986	41.085	1.00	40.49
ATOM	2140	CD2	TYR	C1102	32.609	35.932	42.296	1.00	40.20
ATOM	2141	CE1	TYR	C1102	32.107	38.642	42.061	1.00	41.47
ATOM	2142	CE2	TYR	C1102	31.904	36.580	43.294	1.00	41.62
ATOM	2143	CZ	TYR	C1102	31.672	37.936	43.168	1.00	42.72
ATOM	2144	OH	TYR	C1102	30.961	38.602	44.148	1.00	42.88
ATOM	2145	N	VAL	C1103	36.753	35.276	38.570	1.00	40.18
ATOM	2146	CA	VAL	C1103	37.580	34.400	37.772	1.00	38.79
ATOM	2147	C	VAL	C1103	38.963	35.061	37.561	1.00	40.96
ATOM	2148	O	VAL	C1103	39.070	36.083	36.864	1.00	41.22
ATOM	2149	CB	VAL	C1103	37.038	34.042	36.390	1.00	39.03
ATOM	2150	CG1	VAL	C1103	37.961	33.001	35.738	1.00	35.66
ATOM	2151	CG2	VAL	C1103	35.597	33.463	36.439	1.00	36.18
ATOM	2152	N	ASN	C1104	39.993	34.484	38.154	1.00	41.19
ATOM	2153	CA	ASN	C1104	41.366	34.972	38.131	1.00	43.68
ATOM	2154	C	ASN	C1104	42.006	34.745	36.765	1.00	42.39
ATOM	2155	O	ASN	C1104	42.161	33.569	36.390	1.00	46.58
ATOM	2156	CB	ASN	C1104	42.212	34.184	39.143	1.00	44.69
ATOM	2157	CG	ASN	C1104	43.661	34.686	39.140	1.00	49.43
ATOM	2158	OD1	ASN	C1104	44.630	33.918	38.841	1.00	49.14
ATOM	2159	ND2	ASN	C1104	43.739	35.989	39.460	1.00	47.59
ATOM	2160	N	THR	C1105	42.337	35.771	36.035	1.00	38.71

FIG. 5LL

ATOM	2161	CA	THR	C1105	42.937	35.664	34.723	1.00	38.30
ATOM	2162	C	THR	C1105	44.389	36.105	34.806	1.00	37.67
ATOM	2163	O	THR	C1105	44.998	36.087	33.725	1.00	39.99
ATOM	2164	CB	THR	C1105	42.272	36.465	33.585	1.00	36.40
ATOM	2165	OG1	THR	C1105	42.212	37.883	33.885	1.00	38.39
ATOM	2166	CG2	THR	C1105	40.875	35.906	33.439	1.00	35.66
ATOM	2167	N	THR	C1106	44.918	36.386	35.989	1.00	39.77
ATOM	2168	CA	THR	C1106	46.306	36.915	36.002	1.00	43.19
ATOM	2169	C	THR	C1106	47.368	35.852	36.199	1.00	44.10
ATOM	2170	O	THR	C1106	47.129	34.854	36.896	1.00	45.27
ATOM	2171	CB	THR	C1106	46.445	38.022	37.058	1.00	47.23
ATOM	2172	OG1	THR	C1106	46.210	37.460	38.369	1.00	52.99
ATOM	2173	CG2	THR	C1106	45.403	39.104	36.949	1.00	45.90
ATOM	2174	N	LEU	C1107	48.527	35.962	35.531	1.00	42.56
ATOM	2175	CA	LEU	C1107	49.593	34.961	35.679	1.00	44.02
ATOM	2176	C	LEU	C1107	50.420	35.168	36.946	1.00	46.86
ATOM	2177	O	LEU	C1107	50.888	36.295	37.127	1.00	49.56
ATOM	2178	CB	LEU	C1107	50.539	34.986	34.483	1.00	38.92
ATOM	2179	CG	LEU	C1107	49.970	34.778	33.106	1.00	37.89
ATOM	2180	CD1	LEU	C1107	51.073	34.991	32.082	1.00	39.13
ATOM	2181	CD2	LEU	C1107	49.400	33.350	32.925	1.00	34.26
ATOM	2182	N	TYR	C1108	50.605	34.176	37.803	1.00	49.68
ATOM	2183	CA	TYR	C1108	51.362	34.337	39.032	1.00	53.06
ATOM	2184	C	TYR	C1108	52.666	33.527	38.953	1.00	51.34
ATOM	2185	O	TYR	C1108	53.677	34.091	38.558	1.00	52.57
ATOM	2186	CB	TYR	C1108	50.645	33.861	40.328	1.00	54.61
ATOM	2187	CG	TYR	C1108	49.538	34.857	40.622	1.00	56.02
ATOM	2188	CD1	TYR	C1108	48.208	34.511	40.387	1.00	56.47
ATOM	2189	CD2	TYR	C1108	49.864	36.137	41.055	1.00	56.41
ATOM	2190	CE1	TYR	C1108	47.207	35.441	40.597	1.00	56.50
ATOM	2191	CE2	TYR	C1108	48.864	37.072	41.271	1.00	57.46
ATOM	2192	CZ	TYR	C1108	47.544	36.698	41.044	1.00	57.18
ATOM	2193	OH	TYR	C1108	46.577	37.639	41.267	1.00	58.64
ATOM	2194	N	GLU	C1109	52.585	32.293	39.382	1.00	50.07
ATOM	2195	CA	GLU	C1109	53.718	31.412	39.346	1.00	50.65
ATOM	2196	C	GLU	C1109	53.548	30.323	38.275	1.00	48.97
ATOM	2197	O	GLU	C1109	54.587	29.965	37.719	1.00	47.87
ATOM	2198	CB	GLU	C1109	53.958	30.616	40.626	1.00	53.87
ATOM	2199	CG	GLU	C1109	53.835	31.284	41.965	1.00	58.53
ATOM	2200	CD	GLU	C1109	54.896	32.352	42.202	1.00	60.45
ATOM	2201	OE1	GLU	C1109	56.092	31.991	42.113	1.00	61.68
ATOM	2202	OE2	GLU	C1109	54.482	33.514	42.480	1.00	61.69
ATOM	2203	N	LYS	C1110	52.345	29.727	38.224	1.00	47.13
ATOM	2204	CA	LYS	C1110	52.186	28.577	37.324	1.00	45.74
ATOM	2205	C	LYS	C1110	50.816	28.638	36.645	1.00	42.35
ATOM	2206	O	LYS	C1110	49.924	29.188	37.270	1.00	41.09
ATOM	2207	CB	LYS	C1110	52.400	27.320	38.151	1.00	48.67
ATOM	2208	CG	LYS	C1110	52.564	26.005	37.440	1.00	53.26
ATOM	2209	CD	LYS	C1110	53.174	24.877	38.287	1.00	56.04
ATOM	2210	CE	LYS	C1110	54.685	25.087	38.489	1.00	58.45
ATOM	2211	NZ	LYS	C1110	55.447	23.870	38.929	1.00	58.97
ATOM	2212	N	PHE	C1111	50.666	28.295	35.359	1.00	37.18
ATOM	2213	CA	PHE	C1111	49.325	28.434	34.823	1.00	36.07
ATOM	2214	C	PHE	C1111	49.163	27.464	33.658	1.00	33.65
ATOM	2215	O	PHE	C1111	49.926	27.605	32.736	1.00	31.39
ATOM	2216	CB	PHE	C1111	48.962	29.880	34.438	1.00	36.60
ATOM	2217	CG	PHE	C1111	47.531	30.157	34.143	1.00	37.58

FIG. 5MM

ATOM	2218	CD1	PHE	C1111	46.754	30.911	35.026	1.00	40.75
ATOM	2219	CD2	PHE	C1111	46.914	29.636	33.009	1.00	37.53
ATOM	2220	CE1	PHE	C1111	45.395	31.140	34.795	1.00	40.10
ATOM	2221	CE2	PHE	C1111	45.582	29.887	32.758	1.00	37.72
ATOM	2222	CZ	PHE	C1111	44.824	30.635	33.643	1.00	38.68
ATOM	2223	N	THR	C1112	48.115	26.664	33.719	1.00	28.79
ATOM	2224	CA	THR	C1112	47.688	25.828	32.634	1.00	31.45
ATOM	2225	C	THR	C1112	46.183	26.063	32.377	1.00	30.94
ATOM	2226	O	THR	C1112	45.468	26.129	33.377	1.00	29.01
ATOM	2227	CB	THR	C1112	47.744	24.317	33.099	1.00	32.34
ATOM	2228	OG1	THR	C1112	49.026	24.124	33.723	1.00	35.99
ATOM	2229	CG2	THR	C1112	47.738	23.401	31.909	1.00	32.22
ATOM	2230	N	TYR	C1113	45.708	26.099	31.158	1.00	28.73
ATOM	2231	CA	TYR	C1113	44.309	26.076	30.840	1.00	28.29
ATOM	2232	C	TYR	C1113	43.709	24.640	30.942	1.00	31.34
ATOM	2233	O	TYR	C1113	44.388	23.615	30.928	1.00	25.50
ATOM	2234	CB	TYR	C1113	44.203	26.353	29.330	1.00	27.79
ATOM	2235	CG	TYR	C1113	44.656	27.778	29.016	1.00	29.11
ATOM	2236	CD1	TYR	C1113	45.753	27.954	28.181	1.00	30.15
ATOM	2237	CD2	TYR	C1113	44.032	28.897	29.544	1.00	27.99
ATOM	2238	CE1	TYR	C1113	46.199	29.241	27.868	1.00	31.57
ATOM	2239	CE2	TYR	C1113	44.460	30.198	29.201	1.00	30.17
ATOM	2240	CZ	TYR	C1113	45.571	30.354	28.371	1.00	30.26
ATOM	2241	OH	TYR	C1113	46.068	31.611	28.045	1.00	30.20
ATOM	2242	N	ALA	C1114	42.398	24.636	31.120	1.00	29.12
ATOM	2243	CA	ALA	C1114	41.638	23.395	31.035	1.00	30.29
ATOM	2244	C	ALA	C1114	41.882	22.872	29.625	1.00	30.26
ATOM	2245	O	ALA	C1114	41.791	23.661	28.680	1.00	30.70
ATOM	2246	CB	ALA	C1114	40.127	23.678	31.199	1.00	30.91
ATOM	2247	N	GLY	C1115	42.135	21.544	29.515	1.00	28.43
ATOM	2248	CA	GLY	C1115	42.371	21.045	28.199	1.00	30.36
ATOM	2249	C	GLY	C1115	41.138	20.933	27.334	1.00	34.03
ATOM	2250	O	GLY	C1115	39.913	20.801	27.653	1.00	35.50
ATOM	2251	N	ILE	C1116	41.445	21.017	26.046	1.00	35.79
ATOM	2252	CA	ILE	C1116	40.554	20.877	24.918	1.00	41.16
ATOM	2253	C	ILE	C1116	40.987	19.601	24.199	1.00	48.93
ATOM	2254	CB	ILE	C1116	40.660	21.990	23.877	1.00	40.53
ATOM	2255	CG1	ILE	C1116	40.332	23.381	24.419	1.00	39.34
ATOM	2256	CG2	ILE	C1116	39.797	21.709	22.629	1.00	40.56
ATOM	2257	CD1	ILE	C1116	40.844	24.462	23.474	1.00	39.48
ATOM	2258	N	ASP	C1117	40.096	18.690	23.816	1.00	56.34
ATOM	2259	CA	ASP	C1117	40.671	17.809	22.759	1.00	64.41
ATOM	2260	C	ASP	C1117	39.582	17.226	21.862	1.00	67.05
ATOM	2261	O	ASP	C1117	38.632	16.639	22.384	1.00	66.11
ATOM	2262	CB	ASP	C1117	41.552	16.679	23.243	1.00	66.12
ATOM	2263	CG	ASP	C1117	42.980	17.054	23.608	1.00	68.11
ATOM	2264	OD1	ASP	C1117	43.730	17.676	22.830	1.00	69.52
ATOM	2265	OD2	ASP	C1117	43.216	16.706	24.787	1.00	68.31
ATOM	2266	N	CYS	C1118	39.775	17.421	20.548	1.00	71.27
ATOM	2267	CA	CYS	C1118	38.800	16.948	19.563	1.00	75.06
ATOM	2268	C	CYS	C1118	39.057	17.522	18.165	1.00	77.90
ATOM	2269	CB	CYS	C1118	37.387	17.351	19.997	1.00	74.91
ATOM	2270	N	SER	C1119	38.094	17.334	17.244	1.00	81.20
ATOM	2271	CA	SER	C1119	38.055	17.960	15.924	1.00	83.28
ATOM	2272	C	SER	C1119	37.335	17.232	14.787	1.00	84.56
ATOM	2273	O	SER	C1119	37.930	16.898	13.740	1.00	85.44
ATOM	2274	CB	SER	C1119	39.493	18.300	15.476	1.00	83.21

FIG. 5NN

ATOM	2275	N	ALA	C1120	36.028	16.990	14.863	1.00	85.16
ATOM	2276	CA	ALA	C1120	35.171	16.384	13.874	1.00	84.89
ATOM	2277	C	ALA	C1120	34.722	14.957	14.213	1.00	85.19
ATOM	2278	O	ALA	C1120	33.876	14.494	13.396	1.00	85.38
ATOM	2279	CB	ALA	C1120	35.714	16.345	12.447	1.00	84.84
TER									
HETATM	2280	C1	IN3	D	1	27.737	34.907	12.224	1.00 40.84
HETATM	2281	N2	IN3	D	1	28.220	33.661	12.185	1.00 40.67
HETATM	2282	C3	IN3	D	1	27.362	32.629	12.233	1.00 40.61
HETATM	2283	C4	IN3	D	1	25.970	32.787	12.323	1.00 41.94
HETATM	2284	C5	IN3	D	1	25.529	34.130	12.362	1.00 41.03
HETATM	2285	N6	IN3	D	1	26.428	35.160	12.315	1.00 40.65
HETATM	2287	N8	IN3	D	1	27.727	31.299	12.203	1.00 42.23
HETATM	2288	C9	IN3	D	1	26.517	30.664	12.312	1.00 42.50
HETATM	2289	C10	IN3	D	1	25.373	31.506	12.348	1.00 44.61
HETATM	2291	N12	IN3	D	1	24.231	34.490	12.467	1.00 43.99
HETATM	2292	C13	IN3	D	1	23.932	30.977	12.436	1.00 47.57
HETATM	2293	C14	IN3	D	1	29.096	30.727	12.190	1.00 42.52
HETATM	2294	C15	IN3	D	1	22.960	31.497	13.194	1.00 50.46
HETATM	2295	C16	IN3	D	1	21.667	30.935	13.250	1.00 51.20
HETATM	2296	C17	IN3	D	1	21.337	29.804	12.531	1.00 51.31
HETATM	2297	C18	IN3	D	1	22.357	29.258	11.751	1.00 51.58
HETATM	2298	C19	IN3	D	1	23.637	29.839	11.712	1.00 51.00
HETATM	2302	N23	IN3	D	1	20.099	29.245	12.581	1.00 52.79
HETATM	2303	S24	IN3	D	1	19.137	29.209	13.847	1.00 53.21
HETATM	2304	O25	IN3	D	1	19.809	29.557	15.058	1.00 54.86
HETATM	2305	O26	IN3	D	1	18.402	27.997	13.940	1.00 52.02
HETATM	2306	C27	IN3	D	1	17.984	30.563	13.554	1.00 59.14
HETATM	2307	C28	IN3	D	1	17.058	30.555	12.515	1.00 62.44
HETATM	2308	C29	IN3	D	1	16.171	31.631	12.344	1.00 63.41
HETATM	2309	C30	IN3	D	1	16.219	32.721	13.201	1.00 61.99
HETATM	2310	C31	IN3	D	1	17.146	32.728	14.233	1.00 61.19
HETATM	2311	C32	IN3	D	1	18.012	31.655	14.412	1.00 59.69
HETATM	2312	CL33	IN3	D	1	17.000	29.190	11.437	1.00 72.20
HETATM	2313	CL34	IN3	D	1	14.971	31.634	11.070	1.00 66.32
HETATM	2317	F38	IN3	D	1	22.188	28.164	10.970	1.00 50.23
HETATM	2318	C39	IN3	D	1	29.429	30.465	13.689	1.00 41.55
HETATM	2319	C40	IN3	D	1	30.719	29.713	13.975	1.00 41.76
HETATM	2320	C41	IN3	D	1	30.922	28.491	13.060	1.00 42.34
HETATM	2321	C42	IN3	D	1	30.611	28.800	11.579	1.00 44.10
HETATM	2322	C43	IN3	D	1	29.231	29.447	11.376	1.00 43.74
HETATM	2331	C52	IN3	D	1	32.457	27.054	14.408	1.00 40.98
HETATM	2332	C53	IN3	D	1	33.702	26.161	14.218	1.00 39.93
HETATM	2333	N54	IN3	D	1	34.865	27.024	14.047	1.00 40.92
HETATM	2334	C55	IN3	D	1	34.719	27.865	12.858	1.00 41.55
HETATM	2335	C56	IN3	D	1	33.437	28.707	12.946	1.00 41.49
HETATM	2336	N57	IN3	D	1	32.249	27.891	13.211	1.00 41.23
HETATM	2346	C67	IN3	D	1	36.230	26.430	14.126	1.00 38.95
TER									
ATOM	2355	O	HOH	W	1	31.108	33.861	12.284	1.00 32.88
ATOM	2356	O	HOH	W	2	26.872	17.118	31.780	1.00 27.53
ATOM	2357	O	HOH	W	3	33.552	31.769	15.218	1.00 24.69
ATOM	2358	O	HOH	W	4	47.567	25.314	28.603	1.00 31.73
ATOM	2359	O	HOH	W	5	2.429	17.063	30.925	1.00 30.32
ATOM	2360	O	HOH	W	7	33.908	23.176	25.246	1.00 32.79
ATOM	2361	O	HOH	W	8	16.942	20.674	27.837	1.00 29.27
ATOM	2362	O	HOH	W	9	41.194	27.270	31.243	1.00 27.50

FIG. 500

ATOM	2363	O	HOH	W	10	36.797	18.417	32.828	1.00	30.03
ATOM	2364	O	HOH	W	11	28.851	18.044	36.031	1.00	31.02
ATOM	2365	O	HOH	W	12	15.509	25.207	20.371	1.00	36.36
ATOM	2366	O	HOH	W	13	9.416	22.554	31.309	1.00	34.74
ATOM	2367	O	HOH	W	14	24.583	41.060	16.124	1.00	44.69
ATOM	2368	O	HOH	W	15	7.357	41.316	15.797	1.00	65.05
ATOM	2369	O	HOH	W	16	40.089	39.018	35.286	1.00	43.58
ATOM	2370	O	HOH	W	17	42.573	39.050	31.498	1.00	33.36
ATOM	2371	O	HOH	W	18	18.935	40.500	18.279	1.00	34.03
ATOM	2372	O	HOH	W	19	13.481	27.068	41.482	1.00	45.27
ATOM	2373	O	HOH	W	20	19.798	23.284	27.046	1.00	32.39
ATOM	2374	O	HOH	W	22	13.750	26.546	29.238	1.00	33.61
ATOM	2375	O	HOH	W	23	15.599	37.531	37.224	1.00	41.73
ATOM	2376	O	HOH	W	24	45.162	20.392	30.028	1.00	51.51
ATOM	2377	O	HOH	W	25	33.164	26.427	17.812	1.00	30.96
ATOM	2378	O	HOH	W	27	25.096	40.967	30.617	1.00	31.07
ATOM	2379	O	HOH	W	28	44.306	23.553	33.708	1.00	44.45
ATOM	2380	O	HOH	W	29	14.071	17.249	33.601	1.00	32.43
ATOM	2381	O	HOH	W	30	30.157	24.039	23.053	1.00	31.23
ATOM	2382	O	HOH	W	31	21.111	43.623	15.597	1.00	74.93
ATOM	2383	O	HOH	W	33	19.327	17.632	28.859	1.00	33.09
ATOM	2384	O	HOH	W	34	13.241	23.665	39.267	1.00	41.89
ATOM	2385	O	HOH	W	35	31.519	44.776	18.549	1.00	43.36
ATOM	2386	O	HOH	W	36	34.470	39.819	38.307	1.00	52.30
ATOM	2387	O	HOH	W	37	19.740	20.765	27.651	1.00	65.54
ATOM	2388	O	HOH	W	38	44.917	36.546	20.426	1.00	59.90
ATOM	2389	O	HOH	W	40	17.011	9.839	35.866	1.00	47.22
ATOM	2390	O	HOH	W	41	38.945	20.370	30.087	1.00	25.50
ATOM	2391	O	HOH	W	43	46.179	22.872	28.085	1.00	39.76
ATOM	2392	O	HOH	W	44	33.414	46.660	18.569	1.00	52.18
ATOM	2393	O	HOH	W	45	25.781	19.393	41.795	1.00	39.77
ATOM	2394	O	HOH	W	46	25.879	14.880	30.825	1.00	26.83
ATOM	2395	O	HOH	W	47	12.674	31.920	35.287	1.00	41.22
ATOM	2396	O	HOH	W	48	36.038	20.519	22.613	1.00	40.75
ATOM	2397	O	HOH	W	49	9.232	35.876	28.692	1.00	40.36
ATOM	2398	O	HOH	W	50	36.218	20.561	20.320	1.00	41.55
ATOM	2399	O	HOH	W	54	27.796	43.597	11.505	1.00	56.18
ATOM	2400	O	HOH	W	56	43.257	28.114	21.417	1.00	40.56
ATOM	2401	O	HOH	W	57	42.324	44.229	29.443	1.00	56.40
ATOM	2402	O	HOH	W	58	31.439	22.023	21.413	1.00	32.43
ATOM	2403	O	HOH	W	59	49.313	32.007	37.867	1.00	46.71
ATOM	2404	O	HOH	W	60	14.875	35.132	15.522	1.00	39.98
ATOM	2405	O	HOH	W	62	20.722	5.005	29.475	1.00	39.73
ATOM	2406	O	HOH	W	63	45.974	43.256	29.290	1.00	41.18
ATOM	2407	O	HOH	W	64	42.241	38.248	37.028	1.00	43.70
ATOM	2408	O	HOH	W	65	32.550	42.002	39.832	1.00	36.99
ATOM	2409	O	HOH	W	67	39.110	46.531	21.311	1.00	37.71
ATOM	2410	O	HOH	W	68	24.108	20.905	21.953	1.00	53.77
ATOM	2411	O	HOH	W	69	1.460	21.994	31.199	1.00	37.30
ATOM	2412	O	HOH	W	70	49.466	21.211	34.770	1.00	51.34
ATOM	2413	O	HOH	W	71	36.003	21.023	42.825	1.00	40.91
ATOM	2414	O	HOH	W	73	22.188	25.684	4.901	1.00	54.10
ATOM	2415	O	HOH	W	74	39.079	46.157	42.492	1.00	62.53
ATOM	2416	O	HOH	W	75	40.067	30.895	33.482	1.00	47.79
ATOM	2417	O	HOH	W	76	46.668	20.370	34.397	1.00	41.58
ATOM	2418	O	HOH	W	78	11.682	32.018	39.657	1.00	44.53
ATOM	2419	O	HOH	W	79	20.567	30.929	42.014	1.00	56.17

ATOM	2420	O	HOH	W	80	22.313	16.019	43.949	1.00	47.96
ATOM	2421	O	HOH	W	83	33.379	32.767	48.175	1.00	44.70
ATOM	2422	O	HOH	W	84	28.448	47.110	11.329	1.00	72.32
ATOM	2423	O	HOH	W	85	11.988	40.527	14.366	1.00	57.96
ATOM	2424	O	HOH	W	86	11.100	37.338	30.951	1.00	55.75
ATOM	2425	O	HOH	W	87	32.424	25.662	10.927	1.00	60.85
ATOM	2426	O	HOH	W	88	40.553	21.024	36.981	1.00	56.71
ATOM	2427	O	HOH	W	89	20.806	40.663	41.692	1.00	49.92
ATOM	2428	O	HOH	W	90	23.126	21.071	24.679	1.00	28.98
ATOM	2429	O	HOH	W	91	21.847	27.668	22.076	1.00	39.04
ATOM	2430	O	HOH	W	92	17.442	12.682	22.568	1.00	42.46
ATOM	2431	O	HOH	W	94	10.365	22.725	38.862	1.00	42.24
ATOM	2432	O	HOH	W	96	12.915	13.110	35.504	1.00	43.57
ATOM	2433	O	HOH	W	97	11.437	18.561	35.709	1.00	49.64
ATOM	2434	O	HOH	W	98	18.202	17.009	21.807	1.00	60.40
ATOM	2435	O	HOH	W	99	13.090	22.057	22.029	1.00	44.65
ATOM	2436	O	HOH	W	100	13.782	3.003	30.101	1.00	45.94
ATOM	2437	O	HOH	W	101	37.114	30.510	14.091	1.00	54.40
ATOM	2438	O	HOH	W	102	39.281	19.995	32.505	1.00	38.67
ATOM	2439	O	HOH	W	103	19.163	41.538	33.907	1.00	49.16
ATOM	2440	O	HOH	W	105	8.161	24.650	30.444	1.00	38.87
ATOM	2441	O	HOH	W	106	19.044	34.146	43.247	1.00	36.17
ATOM	2442	O	HOH	W	107	52.411	29.944	20.957	1.00	47.78
ATOM	2443	O	HOH	W	109	40.926	37.945	21.207	1.00	57.61
ATOM	2444	O	HOH	W	110	23.910	22.805	45.525	1.00	56.43
ATOM	2445	O	HOH	W	111	23.876	43.384	19.810	1.00	29.77
ATOM	2446	O	HOH	W	112	6.751	36.672	21.579	1.00	62.88
ATOM	2447	O	HOH	W	113	43.463	27.806	35.372	1.00	49.32
ATOM	2448	O	HOH	W	114	33.230	32.283	12.794	1.00	37.37
ATOM	2449	O	HOH	W	115	39.120	18.996	40.839	1.00	82.49
ATOM	2450	O	HOH	W	116	17.786	13.772	37.357	1.00	49.91
ATOM	2451	O	HOH	W	117	20.655	9.465	38.822	1.00	43.82
ATOM	2452	O	HOH	W	118	7.544	39.794	24.678	1.00	56.43
ATOM	2453	O	HOH	W	119	34.363	21.476	9.358	1.00	64.39
ATOM	2454	O	HOH	W	120	14.923	37.925	31.147	1.00	51.98
ATOM	2455	O	HOH	W	121	14.386	25.644	36.407	1.00	47.28
ATOM	2456	O	HOH	W	122	33.578	21.114	23.402	1.00	36.98
ATOM	2457	O	HOH	W	123	42.616	19.765	31.993	1.00	46.67
ATOM	2458	O	HOH	W	124	0.324	31.122	29.775	1.00	85.67
ATOM	2459	O	HOH	W	125	44.223	21.073	33.792	1.00	58.84
ATOM	2460	O	HOH	W	126	13.220	29.507	33.957	1.00	42.26
ATOM	2461	O	HOH	W	127	24.661	6.250	44.308	1.00	53.58
ATOM	2462	O	HOH	W	130	37.555	26.025	18.301	1.00	50.21
ATOM	2463	O	HOH	W	131	29.409	15.521	23.790	1.00	37.37
ATOM	2464	O	HOH	W	134	37.198	41.960	35.518	1.00	40.19
ATOM	2465	O	HOH	W	135	38.741	36.516	21.186	1.00	31.33
ATOM	2466	O	HOH	W	136	20.039	45.048	11.998	1.00	67.09
ATOM	2467	O	HOH	W	137	44.865	39.383	33.992	1.00	42.87
ATOM	2468	O	HOH	W	138	47.499	41.543	34.693	1.00	41.95
ATOM	2469	O	HOH	W	139	14.470	39.588	29.214	1.00	39.88
ATOM	2470	O	HOH	W	140	25.148	21.128	18.186	1.00	55.16
ATOM	2471	O	HOH	W	141	19.506	9.850	24.839	1.00	56.90
ATOM	2472	O	HOH	W	142	39.082	7.569	29.845	1.00	50.85
ATOM	2473	O	HOH	W	143	37.915	8.580	37.497	1.00	73.18
ATOM	2474	O	HOH	W	144	37.234	11.075	36.059	1.00	55.17
ATOM	2475	O	HOH	W	145	18.909	16.767	43.975	1.00	45.07
ATOM	2476	O	HOH	W	146	53.564	36.062	20.842	1.00	35.39

ATOM	2477	O	HOH W 147	21.172	42.848	12.347	1.00	52.85
TER								

FIG. 5RR

ATOM	1	N	VAL	A	818	77.717	45.877	1.677	1.00100.00
ATOM	2	CA	VAL	A	818	76.698	46.966	1.561	1.00100.00
ATOM	3	C	VAL	A	818	75.278	46.411	1.674	1.00100.00
ATOM	4	O	VAL	A	818	74.803	46.162	2.781	1.00100.00
ATOM	5	CB	VAL	A	818	76.875	47.697	0.239	1.00 68.23
ATOM	9	N	LEU	A	819	74.617	46.228	0.530	1.00100.00
ATOM	10	CA	LEU	A	819	73.248	45.707	0.456	1.00100.00
ATOM	11	C	LEU	A	819	72.629	45.997	-0.918	1.00100.00
ATOM	12	O	LEU	A	819	71.622	46.689	-1.003	1.00100.00
ATOM	13	CB	LEU	A	819	72.369	46.345	1.536	1.00100.00
ATOM	14	CG	LEU	A	819	70.873	46.053	1.525	1.00100.00
ATOM	15	CD1	LEU	A	819	70.592	44.975	2.511	1.00100.00
ATOM	16	CD2	LEU	A	819	70.078	47.283	1.865	1.00100.00
ATOM	18	N	ASP	A	820	73.234	45.474	-1.984	1.00100.00
ATOM	19	CA	ASP	A	820	72.753	45.676	-3.359	1.00100.00
ATOM	20	C	ASP	A	820	71.292	46.104	-3.464	1.00100.00
ATOM	21	O	ASP	A	820	70.399	45.421	-2.983	1.00100.00
ATOM	22	CB	ASP	A	820	72.969	44.396	-4.177	1.00 99.21
ATOM	23	CG	ASP	A	820	71.872	44.160	-5.218	1.00 99.21
ATOM	24	OD1	ASP	A	820	71.584	42.982	-5.509	1.00 99.21
ATOM	25	OD2	ASP	A	820	71.303	45.140	-5.750	1.00 99.21
ATOM	27	N	TRP	A	821	71.050	47.227	-4.126	1.00 93.11
ATOM	28	CA	TRP	A	821	69.694	47.719	-4.268	1.00 93.11
ATOM	29	C	TRP	A	821	68.716	46.617	-4.650	1.00 93.11
ATOM	30	O	TRP	A	821	67.904	46.199	-3.849	1.00 93.11
ATOM	31	CB	TRP	A	821	69.639	48.863	-5.283	1.00 97.87
ATOM	32	CG	TRP	A	821	68.703	49.927	-4.847	1.00 97.87
ATOM	33	CD1	TRP	A	821	68.605	50.452	-3.597	1.00 97.87
ATOM	34	CD2	TRP	A	821	67.667	50.542	-5.622	1.00 97.87
ATOM	35	NE1	TRP	A	821	67.567	51.352	-3.537	1.00 97.87
ATOM	36	CE2	TRP	A	821	66.974	51.429	-4.766	1.00 97.87
ATOM	37	CE3	TRP	A	821	67.255	50.429	-6.949	1.00 97.87
ATOM	38	CZ2	TRP	A	821	65.897	52.197	-5.193	1.00 97.87
ATOM	39	CZ3	TRP	A	821	66.180	51.192	-7.374	1.00 97.87
ATOM	40	CH2	TRP	A	821	65.512	52.065	-6.496	1.00 97.87
ATOM	43	N	ASN	A	822	68.798	46.140	-5.896	1.00100.00
ATOM	44	CA	ASN	A	822	67.901	45.077	-6.364	1.00100.00
ATOM	45	C	ASN	A	822	67.686	43.985	-5.314	1.00100.00
ATOM	46	O	ASN	A	822	66.545	43.614	-5.030	1.00100.00
ATOM	47	CB	ASN	A	822	68.462	44.410	-7.624	1.00 56.29
ATOM	48	CG	ASN	A	822	68.707	42.917	-7.427	1.00 56.29
ATOM	49	OD1	ASN	A	822	69.755	42.499	-6.902	1.00 56.29
ATOM	50	OD2	ASN	A	822	67.739	42.114	-7.837	1.00 56.29
ATOM	54	N	ASP	A	823	68.799	43.469	-4.776	1.00 99.96
ATOM	55	CA	ASP	A	823	68.825	42.413	-3.756	1.00 99.96
ATOM	56	C	ASP	A	823	67.823	42.654	-2.650	1.00 99.96
ATOM	57	O	ASP	A	823	67.545	41.765	-1.846	1.00 99.96
ATOM	58	CB	ASP	A	823	70.218	42.308	-3.153	1.00100.00
ATOM	60	N	ILE	A	824	67.303	43.875	-2.605	1.00 80.08
ATOM	61	CA	ILE	A	824	66.315	44.270	-1.616	1.00 80.08
ATOM	62	C	ILE	A	824	64.958	44.392	-2.274	1.00 80.08
ATOM	63	O	ILE	A	824	64.703	45.359	-2.973	1.00 80.08
ATOM	64	CB	ILE	A	824	66.651	45.641	-0.992	1.00100.00
ATOM	65	CG1	ILE	A	824	67.806	45.506	0.009	1.00100.00
ATOM	66	CG2	ILE	A	824	65.417	46.206	-0.307	1.00100.00
ATOM	67	CD1	ILE	A	824	69.048	44.906	-0.577	1.00100.00

FIG. 6A

ATOM	69	N	LYS	A	825	64.098	43.404	-2.036	1.00	99.67
ATOM	70	CA	LYS	A	825	62.735	43.391	-2.580	1.00	99.67
ATOM	71	C	LYS	A	825	61.938	44.544	-1.938	1.00	99.67
ATOM	72	O	LYS	A	825	61.130	44.334	-1.027	1.00	99.67
ATOM	73	CB	LYS	A	825	62.056	42.021	-2.286	1.00	63.59
ATOM	75	N	PHE	A	826	62.171	45.762	-2.420	1.00	69.32
ATOM	76	CA	PHE	A	826	61.502	46.933	-1.875	1.00	69.32
ATOM	77	C	PHE	A	826	59.977	46.823	-1.994	1.00	69.32
ATOM	78	O	PHE	A	826	59.500	45.922	-2.684	1.00	69.32
ATOM	79	CB	PHE	A	826	62.060	48.158	-2.587	1.00	99.11
ATOM	80	CG	PHE	A	826	63.558	48.351	-2.376	1.00	99.11
ATOM	81	CD1	PHE	A	826	64.470	47.961	-3.343	1.00	99.11
ATOM	82	CD2	PHE	A	826	64.045	48.959	-1.215	1.00	99.11
ATOM	83	CE1	PHE	A	826	65.839	48.178	-3.157	1.00	99.11
ATOM	84	CE2	PHE	A	826	65.418	49.179	-1.027	1.00	99.11
ATOM	85	CZ	PHE	A	826	66.307	48.791	-1.995	1.00	99.11
ATOM	87	N	GLN	A	827	59.222	47.691	-1.307	1.00	70.60
ATOM	88	CA	GLN	A	827	57.728	47.659	-1.347	1.00	70.60
ATOM	89	C	GLN	A	827	57.010	49.023	-1.173	1.00	70.60
ATOM	90	O	GLN	A	827	57.401	49.946	-1.874	1.00	70.60
ATOM	91	CB	GLN	A	827	57.178	46.624	-0.337	1.00	100.00
ATOM	92	CG	GLN	A	827	57.627	45.151	-0.598	1.00	100.00
ATOM	93	CD	GLN	A	827	56.797	44.413	-1.665	1.00	100.00
ATOM	94	OE1	GLN	A	827	55.642	44.036	-1.433	1.00	100.00
ATOM	95	NE2	GLN	A	827	57.396	44.196	-2.831	1.00	100.00
ATOM	99	N	ASP	A	828	56.000	49.149	-0.278	1.00	99.97
ATOM	100	CA	ASP	A	828	55.218	50.418	-0.055	1.00	99.97
ATOM	101	C	ASP	A	828	55.490	51.355	1.163	1.00	99.97
ATOM	102	O	ASP	A	828	56.284	51.045	2.038	1.00	99.97
ATOM	103	CB	ASP	A	828	53.723	50.128	0.010	1.00	100.00
ATOM	104	CG	ASP	A	828	53.034	50.839	1.214	1.00	100.00
ATOM	105	OD1	ASP	A	828	52.702	52.037	1.109	1.00	100.00
ATOM	106	OD2	ASP	A	828	52.834	50.215	2.280	1.00	100.00
ATOM	108	N	VAL	A	829	54.787	52.494	1.212	1.00	100.00
ATOM	109	CA	VAL	A	829	54.900	53.488	2.295	1.00	100.00
ATOM	110	C	VAL	A	829	54.384	53.014	3.639	1.00	100.00
ATOM	111	O	VAL	A	829	53.683	52.012	3.703	1.00	100.00
ATOM	112	CB	VAL	A	829	54.162	54.786	1.912	1.00	100.00
ATOM	114	N	ILE	A	830	54.726	53.770	4.695	1.00	76.50
ATOM	115	CA	ILE	A	830	54.342	53.500	6.102	1.00	76.50
ATOM	116	C	ILE	A	830	53.685	54.717	6.782	1.00	76.50
ATOM	117	O	ILE	A	830	52.464	54.830	6.808	1.00	76.50
ATOM	118	CB	ILE	A	830	55.571	53.069	6.979	1.00	83.02
ATOM	119	CG1	ILE	A	830	55.888	51.607	6.755	1.00	83.02
ATOM	120	CG2	ILE	A	830	55.269	53.185	8.437	1.00	83.02
ATOM	121	CD1	ILE	A	830	57.118	51.163	7.437	1.00	83.02
ATOM	123	N	GLY	A	831	54.492	55.626	7.327	1.00	100.00
ATOM	124	CA	GLY	A	831	53.930	56.779	8.009	1.00	100.00
ATOM	125	C	GLY	A	831	54.664	58.090	7.811	1.00	100.00
ATOM	126	O	GLY	A	831	54.659	58.963	8.677	1.00	100.00
ATOM	128	N	GLU	A	832	55.301	58.216	6.660	1.00	46.31
ATOM	129	CA	GLU	A	832	56.045	59.418	6.271	1.00	46.31
ATOM	130	C	GLU	A	832	57.586	59.215	6.265	1.00	46.31
ATOM	131	O	GLU	A	832	58.101	58.149	5.892	1.00	46.31
ATOM	132	CB	GLU	A	832	55.668	60.618	7.158	1.00	100.00
ATOM	133	CG	GLU	A	832	54.587	61.531	6.557	1.00	100.00
ATOM	134	CD	GLU	A	832	54.197	62.702	7.473	1.00	100.00

FIG. 6B

ATOM	135	OE1	GLU	A	832	52.980	62.942	7.660	1.00100.00
ATOM	136	OE2	GLU	A	832	55.107	63.387	8.002	1.00100.00
ATOM	138	N	GLY	A	833	58.330	60.239	6.650	1.00100.00
ATOM	139	CA	GLY	A	833	59.762	60.092	6.672	1.00100.00
ATOM	140	C	GLY	A	833	60.311	61.410	7.090	1.00100.00
ATOM	141	O	GLY	A	833	60.675	61.601	8.251	1.00100.00
ATOM	143	N	ASN	A	834	60.339	62.327	6.130	1.00 87.28
ATOM	144	CA	ASN	A	834	60.829	63.680	6.360	1.00 87.28
ATOM	145	C	ASN	A	834	62.306	63.520	6.639	1.00 87.28
ATOM	146	O	ASN	A	834	62.684	62.859	7.613	1.00 87.28
ATOM	147	CB	ASN	A	834	60.114	64.306	7.570	1.00100.00
ATOM	148	CG	ASN	A	834	60.641	65.685	7.932	1.00100.00
ATOM	149	OD1	ASN	A	834	61.822	65.865	8.248	1.00100.00
ATOM	150	ND2	ASN	A	834	59.751	66.671	7.903	1.00100.00
ATOM	154	N	PHE	A	835	63.131	64.125	5.782	1.00 68.16
ATOM	155	CA	PHE	A	835	64.561	64.036	5.925	1.00 68.16
ATOM	156	C	PHE	A	835	64.700	62.693	6.578	1.00 68.16
ATOM	157	O	PHE	A	835	65.138	62.586	7.733	1.00 68.16
ATOM	158	CB	PHE	A	835	65.073	65.139	6.840	1.00 80.78
ATOM	159	CG	PHE	A	835	65.317	66.447	6.135	1.00 80.78
ATOM	160	CD1	PHE	A	835	64.950	67.651	6.733	1.00 80.78
ATOM	161	CD2	PHE	A	835	65.931	66.475	4.877	1.00 80.78
ATOM	162	CE1	PHE	A	835	65.190	68.856	6.097	1.00 80.78
ATOM	163	CE2	PHE	A	835	66.178	67.689	4.226	1.00 80.78
ATOM	164	CZ	PHE	A	835	65.805	68.881	4.838	1.00 80.78
ATOM	166	N	GLY	A	836	64.226	61.691	5.832	1.00100.00
ATOM	167	CA	GLY	A	836	64.252	60.304	6.257	1.00100.00
ATOM	168	C	GLY	A	836	62.962	59.578	5.914	1.00100.00
ATOM	169	O	GLY	A	836	62.314	59.012	6.792	1.00100.00
ATOM	171	N	GLN	A	837	62.599	59.565	4.636	1.00 88.37
ATOM	172	CA	GLN	A	837	61.356	58.915	4.214	1.00 88.37
ATOM	173	C	GLN	A	837	61.114	57.472	4.701	1.00 88.37
ATOM	174	O	GLN	A	837	61.739	56.544	4.186	1.00 88.37
ATOM	175	CB	GLN	A	837	61.206	58.983	2.666	1.00 70.59
ATOM	176	CG	GLN	A	837	62.424	58.531	1.876	1.00 70.59
ATOM	177	CD	GLN	A	837	62.484	59.097	0.437	1.00 70.59
ATOM	178	OE1	GLN	A	837	63.560	59.517	-0.041	1.00 70.59
ATOM	179	NE2	GLN	A	837	61.327	59.088	-0.263	1.00 70.59
ATOM	183	N	VAL	A	838	60.211	57.302	5.687	1.00 63.61
ATOM	184	CA	VAL	A	838	59.835	55.959	6.213	1.00 63.61
ATOM	185	C	VAL	A	838	58.710	55.222	5.481	1.00 63.61
ATOM	186	O	VAL	A	838	57.525	55.380	5.807	1.00 63.61
ATOM	187	CB	VAL	A	838	59.384	55.939	7.692	1.00 61.77
ATOM	188	CG1	VAL	A	838	60.243	54.967	8.446	1.00 61.77
ATOM	189	CG2	VAL	A	838	59.418	57.290	8.292	1.00 61.77
ATOM	191	N	LEU	A	839	59.114	54.397	4.520	1.00100.00
ATOM	192	CA	LEU	A	839	58.201	53.584	3.738	1.00100.00
ATOM	193	C	LEU	A	839	58.399	52.107	4.098	1.00100.00
ATOM	194	O	LEU	A	839	59.473	51.694	4.507	1.00100.00
ATOM	195	CB	LEU	A	839	58.464	53.783	2.244	1.00100.00
ATOM	196	CG	LEU	A	839	58.836	55.168	1.719	1.00100.00
ATOM	197	CD1	LEU	A	839	58.069	56.233	2.461	1.00100.00
ATOM	198	CD2	LEU	A	839	60.323	55.367	1.853	1.00100.00
ATOM	200	N	LYS	A	840	57.352	51.315	3.969	1.00 58.16
ATOM	201	CA	LYS	A	840	57.459	49.901	4.259	1.00 58.16
ATOM	202	C	LYS	A	840	58.091	49.174	3.081	1.00 58.16
ATOM	203	O	LYS	A	840	57.837	49.497	1.943	1.00 58.16

FIG. 6C

ATOM	204	CB	LYS	A	840	56.071	49.313	4.549	1.00	67.71
ATOM	205	CG	LYS	A	840	56.075	47.809	4.810	1.00	67.71
ATOM	206	CD	LYS	A	840	55.274	47.391	6.047	1.00	67.71
ATOM	207	CE	LYS	A	840	55.467	45.926	6.360	1.00	67.71
ATOM	208	NZ	LYS	A	840	56.848	45.463	6.017	1.00	67.71
ATOM	213	N	ALA	A	841	58.916	48.176	3.344	1.00	99.75
ATOM	214	CA	ALA	A	841	59.514	47.452	2.241	1.00	99.75
ATOM	215	C	ALA	A	841	59.845	46.037	2.620	1.00	99.75
ATOM	216	O	ALA	A	841	59.830	45.684	3.796	1.00	99.75
ATOM	217	CB	ALA	A	841	60.748	48.152	1.771	1.00	78.22
ATOM	219	N	ARG	A	842	60.143	45.231	1.605	1.00	100.00
ATOM	220	CA	ARG	A	842	60.499	43.832	1.798	1.00	100.00
ATOM	221	C	ARG	A	842	61.972	43.576	1.429	1.00	100.00
ATOM	222	O	ARG	A	842	62.288	43.082	0.352	1.00	100.00
ATOM	223	CB	ARG	A	842	59.574	42.951	0.973	1.00	100.00
ATOM	225	N	ILE	A	843	62.868	43.919	2.348	1.00	100.00
ATOM	226	CA	ILE	A	843	64.301	43.743	2.148	1.00	100.00
ATOM	227	C	ILE	A	843	64.642	42.262	2.174	1.00	100.00
ATOM	228	O	ILE	A	843	63.952	41.488	2.844	1.00	100.00
ATOM	229	CB	ILE	A	843	65.094	44.489	3.263	1.00	99.77
ATOM	230	CG1	ILE	A	843	65.193	45.960	2.907	1.00	99.77
ATOM	231	CG2	ILE	A	843	66.487	43.937	3.421	1.00	99.77
ATOM	232	CD1	ILE	A	843	63.857	46.576	2.554	1.00	99.77
ATOM	234	N	LYS	A	844	65.691	41.882	1.435	1.00	77.20
ATOM	235	CA	LYS	A	844	66.176	40.501	1.379	1.00	77.20
ATOM	236	C	LYS	A	844	67.635	40.390	1.854	1.00	77.20
ATOM	237	O	LYS	A	844	68.499	41.059	1.313	1.00	77.20
ATOM	238	CB	LYS	A	844	66.063	39.973	-0.045	1.00	63.87
ATOM	240	N	LYS	A	845	67.921	39.570	2.859	1.00	93.93
ATOM	241	CA	LYS	A	845	69.313	39.419	3.302	1.00	93.93
ATOM	242	C	LYS	A	845	69.979	38.431	2.382	1.00	93.93
ATOM	243	O	LYS	A	845	69.341	37.931	1.453	1.00	93.93
ATOM	244	CB	LYS	A	845	69.391	38.854	4.684	1.00	20.96
ATOM	246	N	ASP	A	846	71.258	38.140	2.631	1.00	72.18
ATOM	247	CA	ASP	A	846	71.912	37.136	1.815	1.00	72.18
ATOM	248	C	ASP	A	846	70.882	36.018	2.059	1.00	72.18
ATOM	249	O	ASP	A	846	70.861	35.389	3.129	1.00	72.18
ATOM	250	CB	ASP	A	846	73.294	36.787	2.390	1.00	100.00
ATOM	251	CG	ASP	A	846	74.415	37.685	1.842	1.00	100.00
ATOM	252	OD1	ASP	A	846	74.632	37.694	0.607	1.00	100.00
ATOM	253	OD2	ASP	A	846	75.083	38.376	2.650	1.00	100.00
ATOM	255	N	GLY	A	847	69.992	35.836	1.082	1.00	99.53
ATOM	256	CA	GLY	A	847	68.923	34.870	1.231	1.00	99.53
ATOM	257	C	GLY	A	847	68.008	35.367	2.347	1.00	99.53
ATOM	258	O	GLY	A	847	68.509	35.974	3.302	1.00	99.53
ATOM	260	N	LEU	A	848	66.694	35.120	2.228	1.00	93.78
ATOM	261	CA	LEU	A	848	65.670	35.542	3.212	1.00	93.78
ATOM	262	C	LEU	A	848	65.095	36.935	2.949	1.00	93.78
ATOM	263	O	LEU	A	848	65.825	37.878	2.662	1.00	93.78
ATOM	264	CB	LEU	A	848	66.215	35.504	4.654	1.00	100.00
ATOM	265	CG	LEU	A	848	66.931	36.752	5.223	1.00	100.00
ATOM	266	CD1	LEU	A	848	65.937	37.849	5.552	1.00	100.00
ATOM	267	CD2	LEU	A	848	67.719	36.377	6.472	1.00	100.00
ATOM	269	N	ARG	A	849	63.781	37.063	3.070	1.00	80.14
ATOM	270	CA	ARG	A	849	63.127	38.347	2.855	1.00	80.14
ATOM	271	C	ARG	A	849	62.191	38.669	4.013	1.00	80.14
ATOM	272	O	ARG	A	849	61.629	37.748	4.612	1.00	80.14

FIG. 6D

ATOM	273	CB	ARG	A	849	62.320	38.327	1.561	1.00	99.23
ATOM	274	CG	ARG	A	849	61.390	37.148	1.452	1.00	99.23
ATOM	275	CD	ARG	A	849	60.021	37.392	2.081	1.00	99.23
ATOM	276	NE	ARG	A	849	59.022	36.466	1.540	1.00	99.23
ATOM	277	CZ	ARG	A	849	58.743	35.268	2.050	1.00	99.23
ATOM	278	NH1	ARG	A	849	59.379	34.826	3.127	1.00	99.23
ATOM	279	NH2	ARG	A	849	57.830	34.504	1.475	1.00	99.23
ATOM	286	N	MET	A	850	62.041	39.958	4.350	1.00	26.65
ATOM	287	CA	MET	A	850	61.122	40.332	5.425	1.00	26.65
ATOM	288	C	MET	A	850	60.680	41.820	5.406	1.00	26.65
ATOM	289	O	MET	A	850	60.502	42.468	4.345	1.00	26.65
ATOM	290	CB	MET	A	850	61.743	39.999	6.780	1.00	99.56
ATOM	291	CG	MET	A	850	63.156	39.475	6.689	1.00	99.56
ATOM	292	SD	MET	A	850	64.190	40.566	5.745	1.00	99.56
ATOM	293	CE	MET	A	850	65.522	40.771	6.902	1.00	99.56
ATOM	295	N	ASP	A	851	60.515	42.341	6.612	1.00	27.82
ATOM	296	CA	ASP	A	851	60.156	43.721	6.812	1.00	27.82
ATOM	297	C	ASP	A	851	61.331	44.534	7.280	1.00	27.82
ATOM	298	O	ASP	A	851	62.056	44.144	8.255	1.00	27.82
ATOM	299	CB	ASP	A	851	59.124	43.799	7.903	1.00	16.75
ATOM	300	CG	ASP	A	851	58.382	42.570	7.998	1.00	16.75
ATOM	301	OD1	ASP	A	851	58.147	42.049	6.837	1.00	16.75
ATOM	302	OD2	ASP	A	851	58.079	42.189	9.190	1.00	16.75
ATOM	304	N	ALA	A	852	61.420	45.691	6.635	1.00	37.08
ATOM	305	CA	ALA	A	852	62.400	46.719	6.887	1.00	37.08
ATOM	306	C	ALA	A	852	61.643	48.050	6.795	1.00	37.08
ATOM	307	O	ALA	A	852	60.764	48.247	5.950	1.00	37.08
ATOM	308	CB	ALA	A	852	63.471	46.663	5.835	1.00	100.00
ATOM	310	N	ALA	A	853	61.955	48.986	7.663	1.00	97.32
ATOM	311	CA	ALA	A	853	61.303	50.269	7.528	1.00	97.32
ATOM	312	C	ALA	A	853	62.427	51.046	6.852	1.00	97.32
ATOM	313	O	ALA	A	853	63.501	51.201	7.415	1.00	97.32
ATOM	314	CB	ALA	A	853	60.947	50.824	8.895	1.00	15.46
ATOM	316	N	ILE	A	854	62.187	51.469	5.617	1.00	84.85
ATOM	317	CA	ILE	A	854	63.178	52.179	4.810	1.00	84.85
ATOM	318	C	ILE	A	854	63.221	53.682	4.985	1.00	84.85
ATOM	319	O	ILE	A	854	62.197	54.334	5.006	1.00	84.85
ATOM	320	CB	ILE	A	854	62.961	51.895	3.315	1.00	99.86
ATOM	321	CG1	ILE	A	854	63.540	50.538	2.948	1.00	99.86
ATOM	322	CG2	ILE	A	854	63.622	52.963	2.474	1.00	99.86
ATOM	323	CD1	ILE	A	854	63.707	49.610	4.109	1.00	99.86
ATOM	325	N	LYS	A	855	64.426	54.228	5.095	1.00	100.00
ATOM	326	CA	LYS	A	855	64.602	55.666	5.249	1.00	100.00
ATOM	327	C	LYS	A	855	65.867	56.179	4.602	1.00	100.00
ATOM	328	O	LYS	A	855	66.915	55.567	4.710	1.00	100.00
ATOM	329	CB	LYS	A	855	64.640	56.058	6.721	1.00	100.00
ATOM	330	CG	LYS	A	855	65.352	57.373	6.977	1.00	100.00
ATOM	331	CD	LYS	A	855	64.912	57.985	8.283	1.00	100.00
ATOM	332	CE	LYS	A	855	65.371	57.143	9.459	1.00	100.00
ATOM	333	NZ	LYS	A	855	66.801	57.366	9.812	1.00	100.00
ATOM	338	N	ARG	A	856	65.751	57.314	3.927	1.00	100.00
ATOM	339	CA	ARG	A	856	66.881	57.980	3.282	1.00	100.00
ATOM	340	C	ARG	A	856	66.403	59.192	2.543	1.00	100.00
ATOM	341	O	ARG	A	856	65.575	59.088	1.631	1.00	100.00
ATOM	342	CB	ARG	A	856	67.602	57.089	2.279	1.00	100.00
ATOM	343	CG	ARG	A	856	68.637	57.868	1.462	1.00	100.00
ATOM	344	CD	ARG	A	856	68.118	58.410	0.090	1.00	100.00

FIG. 6E

ATOM	345	NE	ARG	A	856	68.946	59.472	-0.512	1.00100.00
ATOM	346	CZ	ARG	A	856	68.938	59.819	-1.801	1.00100.00
ATOM	347	NH1	ARG	A	856	68.145	59.210	-2.674	1.00100.00
ATOM	348	NH2	ARG	A	856	69.744	60.783	-2.222	1.00100.00
ATOM	355	N	MET	A	857	66.951	60.337	2.922	1.00 39.23
ATOM	356	CA	MET	A	857	66.567	61.616	2.275	1.00 39.23
ATOM	357	C	MET	A	857	67.634	62.754	2.130	1.00 39.23
ATOM	358	O	MET	A	857	68.221	63.225	3.157	1.00 39.23
ATOM	359	CB	MET	A	857	65.320	62.179	2.983	1.00100.00
ATOM	360	CG	MET	A	857	64.305	62.877	2.092	1.00100.00
ATOM	361	SD	MET	A	857	63.851	64.409	2.908	1.00100.00
ATOM	362	CE	MET	A	857	61.992	64.355	2.935	1.00100.00
ATOM	363	OXT	MET	A	857	67.842	63.172	0.963	1.00100.00
ATOM	365	N	ASP	A	864	73.761	67.110	-3.548	1.00 99.95
ATOM	366	CA	ASP	A	864	74.976	66.819	-4.360	1.00 99.95
ATOM	367	C	ASP	A	864	76.224	67.493	-3.781	1.00 99.95
ATOM	368	O	ASP	A	864	77.068	68.001	-4.530	1.00 99.95
ATOM	369	CB	ASP	A	864	74.765	67.261	-5.839	1.00 2.00
ATOM	373	N	ASP	A	865	76.338	67.492	-2.453	1.00100.00
ATOM	374	CA	ASP	A	865	77.486	68.080	-1.760	1.00100.00
ATOM	375	C	ASP	A	865	77.219	68.112	-0.267	1.00100.00
ATOM	376	O	ASP	A	865	77.444	69.131	0.391	1.00100.00
ATOM	377	CB	ASP	A	865	77.720	69.454	-2.255	1.00 53.42
ATOM	379	N	HIS	A	866	76.752	66.983	0.263	1.00100.00
ATOM	380	CA	HIS	A	866	76.397	66.853	1.678	1.00100.00
ATOM	381	C	HIS	A	866	76.696	65.441	2.178	1.00100.00
ATOM	382	O	HIS	A	866	75.859	64.777	2.805	1.00100.00
ATOM	383	CB	HIS	A	866	74.905	67.144	1.848	1.00100.00
ATOM	384	CG	HIS	A	866	74.036	66.378	0.896	1.00100.00
ATOM	385	ND1	HIS	A	866	73.693	66.857	-0.350	1.00100.00
ATOM	386	CD2	HIS	A	866	73.459	65.158	1.003	1.00100.00
ATOM	387	CE1	HIS	A	866	72.943	65.965	-0.970	1.00100.00
ATOM	388	NE2	HIS	A	866	72.787	64.925	-0.170	1.00100.00
ATOM	392	N	ARG	A	867	77.912	64.998	1.913	1.00100.00
ATOM	393	CA	ARG	A	867	78.335	63.673	2.300	1.00100.00
ATOM	394	C	ARG	A	867	78.856	63.654	3.738	1.00100.00
ATOM	395	O	ARG	A	867	80.061	63.597	3.985	1.00100.00
ATOM	396	CB	ARG	A	867	79.393	63.206	1.310	1.00 99.71
ATOM	397	CG	ARG	A	867	79.185	63.783	-0.098	1.00 99.71
ATOM	398	CD	ARG	A	867	79.695	65.213	-0.213	1.00 99.71
ATOM	399	NE	ARG	A	867	81.116	65.305	0.115	1.00 99.71
ATOM	400	CZ	ARG	A	867	81.604	65.381	1.351	1.00 99.71
ATOM	401	NH1	ARG	A	867	80.785	65.378	2.396	1.00 99.71
ATOM	402	NH2	ARG	A	867	82.919	65.450	1.540	1.00 99.71
ATOM	409	N	ASP	A	868	77.920	63.713	4.683	1.00 88.85
ATOM	410	CA	ASP	A	868	78.239	63.706	6.112	1.00 88.85
ATOM	411	C	ASP	A	868	77.969	62.278	6.646	1.00 88.85
ATOM	412	O	ASP	A	868	78.558	61.850	7.655	1.00 88.85
ATOM	413	CB	ASP	A	868	77.368	64.758	6.870	1.00 67.57
ATOM	414	CG	ASP	A	868	77.674	66.231	6.460	1.00 67.57
ATOM	415	OD1	ASP	A	868	78.671	66.496	5.753	1.00 67.57
ATOM	416	OD2	ASP	A	868	76.914	67.142	6.852	1.00 67.57
ATOM	418	N	PHE	A	869	77.097	61.545	5.943	1.00100.00
ATOM	419	CA	PHE	A	869	76.719	60.176	6.322	1.00100.00
ATOM	420	C	PHE	A	869	77.809	59.128	6.086	1.00100.00
ATOM	421	O	PHE	A	869	78.433	59.091	5.017	1.00100.00
ATOM	422	CB	PHE	A	869	75.431	59.745	5.595	1.00 98.24

FIG. 6F

ATOM	423	CG	PHE	A	869	75.346	60.207	4.164	1.00	98.24
ATOM	424	CD1	PHE	A	869	74.434	61.186	3.789	1.00	98.24
ATOM	425	CD2	PHE	A	869	76.165	59.652	3.186	1.00	98.24
ATOM	426	CE1	PHE	A	869	74.341	61.604	2.457	1.00	98.24
ATOM	427	CE2	PHE	A	869	76.078	60.063	1.854	1.00	98.24
ATOM	428	CZ	PHE	A	869	75.166	61.038	1.492	1.00	98.24
ATOM	430	N	ALA	A	870	78.007	58.287	7.106	1.00	100.00
ATOM	431	CA	ALA	A	870	79.005	57.205	7.146	1.00	100.00
ATOM	432	C	ALA	A	870	79.570	57.201	8.564	1.00	100.00
ATOM	433	O	ALA	A	870	80.736	56.892	8.807	1.00	100.00
ATOM	434	CB	ALA	A	870	80.131	57.437	6.134	1.00	100.00
ATOM	436	N	GLY	A	871	78.706	57.575	9.490	1.00	100.00
ATOM	437	CA	GLY	A	871	79.058	57.626	10.888	1.00	100.00
ATOM	438	C	GLY	A	871	77.783	57.234	11.591	1.00	100.00
ATOM	439	O	GLY	A	871	77.802	56.636	12.662	1.00	100.00
ATOM	441	N	GLU	A	872	76.656	57.592	10.987	1.00	100.00
ATOM	442	CA	GLU	A	872	75.384	57.210	11.564	1.00	100.00
ATOM	443	C	GLU	A	872	75.581	55.695	11.584	1.00	100.00
ATOM	444	O	GLU	A	872	75.628	55.083	12.655	1.00	100.00
ATOM	445	CB	GLU	A	872	74.200	57.613	10.651	1.00	99.93
ATOM	446	CG	GLU	A	872	73.244	58.668	11.260	1.00	99.93
ATOM	447	CD	GLU	A	872	71.754	58.458	10.919	1.00	99.93
ATOM	448	OE1	GLU	A	872	71.434	57.633	10.040	1.00	99.93
ATOM	449	OE2	GLU	A	872	70.894	59.128	11.532	1.00	99.93
ATOM	451	N	LEU	A	873	75.773	55.121	10.389	1.00	77.06
ATOM	452	CA	LEU	A	873	75.982	53.683	10.215	1.00	77.06
ATOM	453	C	LEU	A	873	77.167	53.198	11.046	1.00	77.06
ATOM	454	O	LEU	A	873	77.384	51.998	11.180	1.00	77.06
ATOM	455	CB	LEU	A	873	76.202	53.366	8.746	1.00	96.97
ATOM	457	N	GLU	A	874	77.920	54.142	11.612	1.00	98.87
ATOM	458	CA	GLU	A	874	79.091	53.832	12.423	1.00	98.87
ATOM	459	C	GLU	A	874	78.740	53.585	13.890	1.00	98.87
ATOM	460	O	GLU	A	874	79.072	52.546	14.449	1.00	98.87
ATOM	461	CB	GLU	A	874	80.107	54.954	12.306	1.00	56.03
ATOM	463	N	VAL	A	875	78.096	54.541	14.543	1.00	100.00
ATOM	464	CA	VAL	A	875	77.725	54.320	15.936	1.00	100.00
ATOM	465	C	VAL	A	875	76.577	53.312	15.875	1.00	100.00
ATOM	466	O	VAL	A	875	76.533	52.370	16.654	1.00	100.00
ATOM	467	CB	VAL	A	875	77.279	55.629	16.582	1.00	100.00
ATOM	469	N	LEU	A	876	75.678	53.520	14.911	1.00	63.64
ATOM	470	CA	LEU	A	876	74.515	52.662	14.649	1.00	63.64
ATOM	471	C	LEU	A	876	74.825	51.155	14.638	1.00	63.64
ATOM	472	O	LEU	A	876	73.935	50.359	14.292	1.00	63.64
ATOM	473	CB	LEU	A	876	73.914	53.005	13.267	1.00	36.83
ATOM	474	CG	LEU	A	876	72.851	54.076	12.997	1.00	36.83
ATOM	475	CD1	LEU	A	876	72.028	53.665	11.807	1.00	36.83
ATOM	476	CD2	LEU	A	876	71.987	54.260	14.181	1.00	36.83
ATOM	478	N	CYS	A	877	76.072	50.786	14.978	1.00	75.85
ATOM	479	CA	CYS	A	877	76.570	49.391	14.973	1.00	75.85
ATOM	480	C	CYS	A	877	76.791	48.697	16.317	1.00	75.85
ATOM	481	O	CYS	A	877	75.965	47.904	16.771	1.00	75.85
ATOM	482	CB	CYS	A	877	77.890	49.343	14.202	1.00	82.25
ATOM	483	SG	CYS	A	877	78.205	50.859	13.250	1.00	82.25
ATOM	485	N	LYS	A	878	77.947	48.968	16.913	1.00	100.00
ATOM	486	CA	LYS	A	878	78.334	48.400	18.202	1.00	100.00
ATOM	487	C	LYS	A	878	77.159	48.295	19.186	1.00	100.00
ATOM	488	O	LYS	A	878	77.237	47.565	20.178	1.00	100.00

ATOM	489	CB	LYS	A	878	79.460	49.251	18.826	1.00	99.60
ATOM	490	CG	LYS	A	878	80.588	49.643	17.842	1.00	99.60
ATOM	491	CD	LYS	A	878	80.814	51.160	17.739	1.00	99.60
ATOM	492	CE	LYS	A	878	81.033	51.598	16.292	1.00	99.60
ATOM	493	NZ	LYS	A	878	82.152	52.567	16.077	1.00	99.60
ATOM	498	N	LEU	A	879	76.079	49.024	18.905	1.00	99.14
ATOM	499	CA	LEU	A	879	74.905	49.034	19.762	1.00	99.14
ATOM	500	C	LEU	A	879	73.664	48.687	18.953	1.00	99.14
ATOM	501	O	LEU	A	879	72.574	48.526	19.488	1.00	99.14
ATOM	502	CB	LEU	A	879	74.748	50.416	20.401	1.00	99.96
ATOM	503	CG	LEU	A	879	74.125	51.546	19.579	1.00	99.96
ATOM	504	CD1	LEU	A	879	74.530	52.863	20.154	1.00	99.96
ATOM	505	CD2	LEU	A	879	74.555	51.454	18.135	1.00	99.96
ATOM	507	N	GLY	A	880	73.840	48.593	17.647	1.00	74.75
ATOM	508	CA	GLY	A	880	72.737	48.256	16.775	1.00	74.75
ATOM	509	C	GLY	A	880	71.778	47.281	17.406	1.00	74.75
ATOM	510	O	GLY	A	880	70.589	47.458	17.285	1.00	74.75
ATOM	512	N	HIS	A	881	72.288	46.243	18.067	1.00	100.00
ATOM	513	CA	HIS	A	881	71.428	45.246	18.700	1.00	100.00
ATOM	514	C	HIS	A	881	71.274	45.583	20.172	1.00	100.00
ATOM	515	O	HIS	A	881	71.798	46.571	20.661	1.00	100.00
ATOM	516	CB	HIS	A	881	71.989	43.818	18.514	1.00	80.74
ATOM	517	CG	HIS	A	881	71.360	42.778	19.401	1.00	80.74
ATOM	518	ND1	HIS	A	881	70.116	42.234	19.155	1.00	80.74
ATOM	519	CD2	HIS	A	881	71.778	42.230	20.573	1.00	80.74
ATOM	520	CE1	HIS	A	881	69.792	41.404	20.133	1.00	80.74
ATOM	521	NE2	HIS	A	881	70.783	41.384	21.007	1.00	80.74
ATOM	525	N	HIS	A	882	70.539	44.718	20.846	1.00	5.03
ATOM	526	CA	HIS	A	882	70.126	44.779	22.266	1.00	5.03
ATOM	527	C	HIS	A	882	68.572	44.646	22.018	1.00	5.03
ATOM	528	O	HIS	A	882	67.998	45.211	20.996	1.00	5.03
ATOM	529	CB	HIS	A	882	70.487	46.161	22.887	1.00	36.20
ATOM	530	CG	HIS	A	882	70.085	46.316	24.322	1.00	36.20
ATOM	531	ND1	HIS	A	882	68.786	46.169	24.753	1.00	36.20
ATOM	532	CD2	HIS	A	882	70.816	46.553	25.432	1.00	36.20
ATOM	533	CE1	HIS	A	882	68.731	46.302	26.066	1.00	36.20
ATOM	534	NE2	HIS	A	882	69.949	46.535	26.504	1.00	36.20
ATOM	538	N	PRO	A	883	67.875	43.928	22.885	1.00	18.79
ATOM	539	CA	PRO	A	883	66.444	43.868	22.564	1.00	18.79
ATOM	540	C	PRO	A	883	65.806	45.252	22.201	1.00	18.79
ATOM	541	O	PRO	A	883	65.014	45.404	21.188	1.00	18.79
ATOM	542	CB	PRO	A	883	65.804	43.294	23.829	1.00	41.14
ATOM	543	CG	PRO	A	883	66.946	43.069	24.810	1.00	41.14
ATOM	544	CD	PRO	A	883	68.231	43.209	24.107	1.00	41.14
ATOM	545	N	ASN	A	884	66.245	46.252	22.975	1.00	21.27
ATOM	546	CA	ASN	A	884	65.656	47.545	22.910	1.00	21.27
ATOM	547	C	ASN	A	884	66.055	48.782	22.174	1.00	21.27
ATOM	548	O	ASN	A	884	65.930	49.811	22.738	1.00	21.27
ATOM	549	CB	ASN	A	884	65.371	47.916	24.332	1.00	47.99
ATOM	550	CG	ASN	A	884	64.926	46.747	25.093	1.00	47.99
ATOM	551	OD1	ASN	A	884	65.360	46.508	26.173	1.00	47.99
ATOM	552	ND2	ASN	A	884	64.056	45.990	24.504	1.00	47.99
ATOM	556	N	ILE	A	885	66.421	48.685	20.906	1.00	2.00
ATOM	557	CA	ILE	A	885	66.784	49.799	20.139	1.00	2.00
ATOM	558	C	ILE	A	885	66.578	49.337	18.712	1.00	2.00
ATOM	559	O	ILE	A	885	67.324	48.601	18.278	1.00	2.00
ATOM	560	CB	ILE	A	885	68.282	50.142	20.404	1.00	5.30

FIG. 6H

ATOM	561	CG1	ILE	A	885	68.387	50.790	21.774	1.00	5.30
ATOM	562	CG2	ILE	A	885	68.946	51.096	19.301	1.00	5.30
ATOM	563	CD1	ILE	A	885	69.834	51.062	22.137	1.00	5.30
ATOM	565	N	ILE	A	886	65.634	49.811	17.931	1.00	41.79
ATOM	566	CA	ILE	A	886	65.528	49.296	16.564	1.00	41.79
ATOM	567	C	ILE	A	886	66.883	48.887	15.937	1.00	41.79
ATOM	568	O	ILE	A	886	67.899	49.217	16.450	1.00	41.79
ATOM	569	CB	ILE	A	886	64.769	50.316	15.671	1.00	97.62
ATOM	570	CG1	ILE	A	886	63.737	49.563	14.817	1.00	97.62
ATOM	571	CG2	ILE	A	886	65.742	51.141	14.871	1.00	97.62
ATOM	572	CD1	ILE	A	886	62.833	50.438	14.004	1.00	97.62
ATOM	574	N	ASN	A	887	66.915	48.190	14.817	1.00	58.02
ATOM	575	CA	ASN	A	887	68.191	47.751	14.300	1.00	58.02
ATOM	576	C	ASN	A	887	68.481	48.230	12.940	1.00	58.02
ATOM	577	O	ASN	A	887	67.635	48.811	12.321	1.00	58.02
ATOM	578	CB	ASN	A	887	68.237	46.228	14.269	1.00	61.11
ATOM	579	CG	ASN	A	887	69.626	45.688	14.460	1.00	61.11
ATOM	580	OD1	ASN	A	887	70.307	45.367	13.505	1.00	61.11
ATOM	581	ND2	ASN	A	887	70.050	45.584	15.711	1.00	61.11
ATOM	585	N	LEU	A	888	69.688	47.945	12.467	1.00	100.00
ATOM	586	CA	LEU	A	888	70.097	48.313	11.122	1.00	100.00
ATOM	587	C	LEU	A	888	70.158	47.037	10.282	1.00	100.00
ATOM	588	O	LEU	A	888	71.039	46.202	10.444	1.00	100.00
ATOM	589	CB	LEU	A	888	71.467	48.993	11.131	1.00	100.00
ATOM	590	CG	LEU	A	888	72.068	49.217	9.743	1.00	100.00
ATOM	591	CD1	LEU	A	888	72.054	50.676	9.410	1.00	100.00
ATOM	592	CD2	LEU	A	888	73.475	48.686	9.699	1.00	100.00
ATOM	594	N	LEU	A	889	69.191	46.880	9.398	1.00	73.18
ATOM	595	CA	LEU	A	889	69.128	45.721	8.530	1.00	73.18
ATOM	596	C	LEU	A	889	70.044	45.860	7.290	1.00	73.18
ATOM	597	O	LEU	A	889	70.737	44.920	6.926	1.00	73.18
ATOM	598	CB	LEU	A	889	67.666	45.500	8.102	1.00	10.03
ATOM	599	CG	LEU	A	889	66.628	44.729	9.010	1.00	10.03
ATOM	600	CD1	LEU	A	889	66.180	43.517	8.146	1.00	10.03
ATOM	601	CD2	LEU	A	889	67.147	44.336	10.432	1.00	10.03
ATOM	603	N	GLY	A	890	70.058	47.028	6.651	1.00	100.00
ATOM	604	CA	GLY	A	890	70.898	47.201	5.475	1.00	100.00
ATOM	605	C	GLY	A	890	71.057	48.582	4.845	1.00	100.00
ATOM	606	O	GLY	A	890	70.515	49.581	5.319	1.00	100.00
ATOM	608	N	ALA	A	891	71.829	48.616	3.758	1.00	93.61
ATOM	609	CA	ALA	A	891	72.124	49.833	2.992	1.00	93.61
ATOM	610	C	ALA	A	891	73.125	49.438	1.929	1.00	93.61
ATOM	611	O	ALA	A	891	73.999	48.626	2.223	1.00	93.61
ATOM	612	CB	ALA	A	891	72.763	50.871	3.886	1.00	28.61
ATOM	614	N	CYS	A	892	73.033	49.985	0.715	1.00	100.00
ATOM	615	CA	CYS	A	892	74.034	49.635	-0.306	1.00	100.00
ATOM	616	C	CYS	A	892	74.789	50.793	-0.956	1.00	100.00
ATOM	617	O	CYS	A	892	75.934	51.073	-0.606	1.00	100.00
ATOM	618	CB	CYS	A	892	73.432	48.787	-1.429	1.00	100.00
ATOM	619	SG	CYS	A	892	74.641	48.356	-2.757	1.00	100.00
ATOM	621	N	GLU	A	893	74.134	51.447	-1.914	1.00	85.23
ATOM	622	CA	GLU	A	893	74.715	52.555	-2.679	1.00	85.23
ATOM	623	C	GLU	A	893	73.816	52.794	-3.880	1.00	85.23
ATOM	624	O	GLU	A	893	74.228	52.512	-5.011	1.00	85.23
ATOM	625	CB	GLU	A	893	76.108	52.176	-3.222	1.00	100.00
ATOM	626	CG	GLU	A	893	77.267	53.065	-2.785	1.00	100.00
ATOM	627	CD	GLU	A	893	78.487	52.246	-2.386	1.00	100.00

FIG. 6I

ATOM	628	OE1	GLU	A	893	79.029	51.535	-3.266	1.00100.00
ATOM	629	OE2	GLU	A	893	78.893	52.307	-1.197	1.00100.00
ATOM	631	N	HIS	A	894	72.602	53.293	-3.664	1.00100.00
ATOM	632	CA	HIS	A	894	71.731	53.508	-4.810	1.00100.00
ATOM	633	C	HIS	A	894	71.825	54.855	-5.463	1.00100.00
ATOM	634	O	HIS	A	894	71.106	55.770	-5.181	1.00100.00
ATOM	635	CB	HIS	A	894	70.261	53.338	-4.477	1.00100.00
ATOM	636	CG	HIS	A	894	69.370	53.597	-5.652	1.00100.00
ATOM	637	ND1	HIS	A	894	68.309	54.476	-5.610	1.00100.00
ATOM	638	CD2	HIS	A	894	69.419	53.128	-6.922	1.00100.00
ATOM	639	CE1	HIS	A	894	67.743	54.539	-6.802	1.00100.00
ATOM	640	NE2	HIS	A	894	68.397	53.729	-7.615	1.00100.00
ATOM	644	N	ARG	A	895	72.888	54.950	-6.340	1.00100.00
ATOM	645	CA	ARG	A	895	73.176	56.161	-7.090	1.00100.00
ATOM	646	C	ARG	A	895	72.331	57.309	-6.481	1.00100.00
ATOM	647	O	ARG	A	895	71.194	57.562	-6.910	1.00100.00
ATOM	648	CB	ARG	A	895	72.842	55.883	-8.571	1.00 36.65
ATOM	649	CG	ARG	A	895	73.711	54.767	-9.229	1.00 36.65
ATOM	650	CD	ARG	A	895	73.012	54.079	-10.421	1.00 36.65
ATOM	651	NE	ARG	A	895	73.587	54.370	-11.738	1.00 36.65
ATOM	652	CZ	ARG	A	895	74.382	53.546	-12.451	1.00 36.65
ATOM	653	NH1	ARG	A	895	74.735	52.315	-11.986	1.00 36.65
ATOM	654	NH2	ARG	A	895	74.848	53.963	-13.644	1.00 36.65
ATOM	661	N	GLY	A	896	72.901	57.979	-5.469	1.00 33.20
ATOM	662	CA	GLY	A	896	72.190	59.016	-4.751	1.00 33.20
ATOM	663	C	GLY	A	896	71.918	58.455	-3.348	1.00 33.20
ATOM	664	O	GLY	A	896	70.779	58.462	-2.847	1.00 33.20
ATOM	666	N	TYR	A	897	72.971	57.947	-2.705	1.00 98.45
ATOM	667	CA	TYR	A	897	72.864	57.372	-1.356	1.00 98.45
ATOM	668	C	TYR	A	897	72.959	55.835	-1.387	1.00 98.45
ATOM	669	O	TYR	A	897	73.599	55.240	-2.258	1.00 98.45
ATOM	670	CB	TYR	A	897	71.532	57.786	-0.716	1.00100.00
ATOM	671	CG	TYR	A	897	71.522	58.208	0.734	1.00100.00
ATOM	672	CD1	TYR	A	897	71.152	59.511	1.080	1.00100.00
ATOM	673	CD2	TYR	A	897	71.631	57.268	1.756	1.00100.00
ATOM	674	CE1	TYR	A	897	70.860	59.866	2.391	1.00100.00
ATOM	675	CE2	TYR	A	897	71.345	57.604	3.074	1.00100.00
ATOM	676	CZ	TYR	A	897	70.947	58.908	3.389	1.00100.00
ATOM	677	OH	TYR	A	897	70.582	59.246	4.682	1.00100.00
ATOM	680	N	LEU	A	898	72.293	55.212	-0.419	1.00100.00
ATOM	681	CA	LEU	A	898	72.272	53.765	-0.258	1.00100.00
ATOM	682	C	LEU	A	898	70.983	53.363	0.469	1.00100.00
ATOM	683	O	LEU	A	898	70.810	52.197	0.836	1.00100.00
ATOM	684	CB	LEU	A	898	73.495	53.328	0.551	1.00 67.92
ATOM	686	N	TYR	A	899	70.097	54.345	0.668	1.00100.00
ATOM	687	CA	TYR	A	899	68.813	54.169	1.347	1.00100.00
ATOM	688	C	TYR	A	899	68.976	53.434	2.680	1.00100.00
ATOM	689	O	TYR	A	899	70.090	53.252	3.153	1.00100.00
ATOM	690	CB	TYR	A	899	67.840	53.420	0.434	1.00 99.94
ATOM	691	CG	TYR	A	899	67.265	54.259	-0.694	1.00 99.94
ATOM	692	CD1	TYR	A	899	67.218	53.770	-2.004	1.00 99.94
ATOM	693	CD2	TYR	A	899	66.738	55.531	-0.454	1.00 99.94
ATOM	694	CE1	TYR	A	899	66.662	54.519	-3.044	1.00 99.94
ATOM	695	CE2	TYR	A	899	66.176	56.295	-1.493	1.00 99.94
ATOM	696	CZ	TYR	A	899	66.143	55.778	-2.780	1.00 99.94
ATOM	697	OH	TYR	A	899	65.580	56.509	-3.792	1.00 99.94
ATOM	700	N	LEU	A	900	67.876	53.017	3.300	1.00 99.32

ATOM	701	CA	LEU	A	900	67.987	52.305	4.573	1.00	99.32
ATOM	702	C	LEU	A	900	67.119	51.071	4.770	1.00	99.32
ATOM	703	O	LEU	A	900	66.306	50.702	3.933	1.00	99.32
ATOM	704	CB	LEU	A	900	67.755	53.258	5.752	1.00	72.65
ATOM	705	CG	LEU	A	900	68.911	53.350	6.752	1.00	72.65
ATOM	706	CD1	LEU	A	900	70.175	52.843	6.059	1.00	72.65
ATOM	707	CD2	LEU	A	900	69.096	54.792	7.259	1.00	72.65
ATOM	709	N	ALA	A	901	67.330	50.439	5.912	1.00	100.00
ATOM	710	CA	ALA	A	901	66.617	49.244	6.288	1.00	100.00
ATOM	711	C	ALA	A	901	66.802	49.053	7.774	1.00	100.00
ATOM	712	O	ALA	A	901	67.774	48.484	8.231	1.00	100.00
ATOM	713	CB	ALA	A	901	67.152	48.049	5.537	1.00	100.00
ATOM	715	N	ILE	A	902	65.840	49.575	8.510	1.00	33.23
ATOM	716	CA	ILE	A	902	65.773	49.510	9.964	1.00	33.23
ATOM	717	C	ILE	A	902	64.912	48.295	10.352	1.00	33.23
ATOM	718	O	ILE	A	902	63.988	47.959	9.648	1.00	33.23
ATOM	719	CB	ILE	A	902	65.130	50.817	10.474	1.00	58.03
ATOM	720	CG1	ILE	A	902	65.930	51.992	9.960	1.00	58.03
ATOM	721	CG2	ILE	A	902	65.107	50.870	11.955	1.00	58.03
ATOM	722	CD1	ILE	A	902	67.193	52.207	10.738	1.00	58.03
ATOM	724	N	GLU	A	903	65.256	47.622	11.440	1.00	37.33
ATOM	725	CA	GLU	A	903	64.468	46.507	11.912	1.00	37.33
ATOM	726	C	GLU	A	903	63.079	47.051	11.790	1.00	37.33
ATOM	727	O	GLU	A	903	62.856	48.198	12.081	1.00	37.33
ATOM	728	CB	GLU	A	903	64.732	46.216	13.388	1.00	74.67
ATOM	729	CG	GLU	A	903	63.667	45.362	14.022	1.00	74.67
ATOM	730	CD	GLU	A	903	63.757	45.302	15.525	1.00	74.67
ATOM	731	OE1	GLU	A	903	62.771	44.921	16.178	1.00	74.67
ATOM	732	OE2	GLU	A	903	64.809	45.637	16.072	1.00	74.67
ATOM	734	N	TYR	A	904	62.137	46.221	11.362	1.00	98.95
ATOM	735	CA	TYR	A	904	60.765	46.667	11.209	1.00	98.95
ATOM	736	C	TYR	A	904	59.912	46.319	12.435	1.00	98.95
ATOM	737	O	TYR	A	904	59.998	45.210	12.968	1.00	98.95
ATOM	738	CB	TYR	A	904	60.187	46.064	9.939	1.00	65.21
ATOM	739	CG	TYR	A	904	58.741	46.366	9.749	1.00	65.21
ATOM	740	CD1	TYR	A	904	58.343	47.461	9.002	1.00	65.21
ATOM	741	CD2	TYR	A	904	57.760	45.602	10.367	1.00	65.21
ATOM	742	CE1	TYR	A	904	56.994	47.797	8.878	1.00	65.21
ATOM	743	CE2	TYR	A	904	56.418	45.929	10.249	1.00	65.21
ATOM	744	CZ	TYR	A	904	56.046	47.029	9.500	1.00	65.21
ATOM	745	OH	TYR	A	904	54.736	47.335	9.321	1.00	65.21
ATOM	748	N	ALA	A	905	59.103	47.287	12.877	1.00	44.07
ATOM	749	CA	ALA	A	905	58.241	47.148	14.049	1.00	44.07
ATOM	750	C	ALA	A	905	56.742	46.973	13.670	1.00	44.07
ATOM	751	O	ALA	A	905	56.091	47.865	13.125	1.00	44.07
ATOM	752	CB	ALA	A	905	58.459	48.326	14.943	1.00	44.16
ATOM	754	N	PRO	A	906	56.169	45.798	13.983	1.00	95.76
ATOM	755	CA	PRO	A	906	54.773	45.513	13.643	1.00	95.76
ATOM	756	C	PRO	A	906	53.627	46.336	14.226	1.00	95.76
ATOM	757	O	PRO	A	906	52.547	46.358	13.656	1.00	95.76
ATOM	758	CB	PRO	A	906	54.642	44.022	13.956	1.00	74.50
ATOM	759	CG	PRO	A	906	55.605	43.816	15.072	1.00	74.50
ATOM	760	CD	PRO	A	906	56.773	44.682	14.734	1.00	74.50
ATOM	761	N	HIS	A	907	53.838	47.018	15.336	1.00	75.88
ATOM	762	CA	HIS	A	907	52.751	47.792	15.909	1.00	75.88
ATOM	763	C	HIS	A	907	52.942	49.300	15.917	1.00	75.88
ATOM	764	O	HIS	A	907	52.370	49.979	16.754	1.00	75.88

FIG. 6K

ATOM	765	CB	HIS	A	907	52.491	47.321	17.327	1.00	58.13
ATOM	766	CG	HIS	A	907	52.494	45.839	17.465	1.00	58.13
ATOM	767	ND1	HIS	A	907	52.400	44.991	16.387	1.00	58.13
ATOM	768	CD2	HIS	A	907	52.595	45.049	18.552	1.00	58.13
ATOM	769	CE1	HIS	A	907	52.442	43.741	16.805	1.00	58.13
ATOM	770	NE2	HIS	A	907	52.563	43.750	18.117	1.00	58.13
ATOM	774	N	GLY	A	908	53.744	49.827	15.004	1.00	99.49
ATOM	775	CA	GLY	A	908	53.952	51.258	14.965	1.00	99.49
ATOM	776	C	GLY	A	908	54.688	51.796	16.168	1.00	99.49
ATOM	777	O	GLY	A	908	55.536	51.126	16.736	1.00	99.49
ATOM	779	N	ASN	A	909	54.345	53.015	16.565	1.00	37.36
ATOM	780	CA	ASN	A	909	54.995	53.672	17.686	1.00	37.36
ATOM	781	C	ASN	A	909	54.274	53.675	18.970	1.00	37.36
ATOM	782	O	ASN	A	909	53.091	53.524	19.093	1.00	37.36
ATOM	783	CB	ASN	A	909	55.422	55.139	17.378	1.00	21.80
ATOM	784	CG	ASN	A	909	54.300	56.174	17.594	1.00	21.80
ATOM	785	OD1	ASN	A	909	54.091	57.036	16.763	1.00	21.80
ATOM	786	ND2	ASN	A	909	53.611	56.094	18.714	1.00	21.80
ATOM	790	N	LEU	A	910	55.043	53.958	19.971	1.00	6.05
ATOM	791	CA	LEU	A	910	54.505	53.895	21.258	1.00	6.05
ATOM	792	C	LEU	A	910	53.372	54.836	21.506	1.00	6.05
ATOM	793	O	LEU	A	910	52.558	54.488	22.290	1.00	6.05
ATOM	794	CB	LEU	A	910	55.629	53.964	22.304	1.00	22.43
ATOM	795	CG	LEU	A	910	55.112	53.756	23.738	1.00	22.43
ATOM	796	CD1	LEU	A	910	54.795	52.285	23.989	1.00	22.43
ATOM	797	CD2	LEU	A	910	56.128	54.383	24.829	1.00	22.43
ATOM	799	N	LEU	A	911	53.269	56.034	20.959	1.00	53.76
ATOM	800	CA	LEU	A	911	52.062	56.772	21.333	1.00	53.76
ATOM	801	C	LEU	A	911	50.801	56.136	20.690	1.00	53.76
ATOM	802	O	LEU	A	911	49.969	55.583	21.406	1.00	53.76
ATOM	803	CB	LEU	A	911	52.158	58.265	20.991	1.00	2.16
ATOM	804	CG	LEU	A	911	51.350	59.370	21.692	1.00	2.16
ATOM	805	CD1	LEU	A	911	51.622	59.513	23.075	1.00	2.16
ATOM	806	CD2	LEU	A	911	51.612	60.569	20.997	1.00	2.16
ATOM	808	N	ASP	A	912	50.566	56.165	19.363	1.00	37.67
ATOM	809	CA	ASP	A	912	49.481	55.594	18.764	1.00	37.67
ATOM	810	C	ASP	A	912	49.087	54.287	19.391	1.00	37.67
ATOM	811	O	ASP	A	912	48.010	54.116	19.875	1.00	37.67
ATOM	812	CB	ASP	A	912	49.652	55.383	17.285	1.00	2.00
ATOM	813	CG	ASP	A	912	49.965	56.675	16.516	1.00	2.00
ATOM	814	OD1	ASP	A	912	49.929	56.718	15.258	1.00	2.00
ATOM	815	OD2	ASP	A	912	50.263	57.647	17.195	1.00	2.00
ATOM	817	N	PHE	A	913	49.977	53.341	19.403	1.00	21.37
ATOM	818	CA	PHE	A	913	49.659	52.056	19.975	1.00	21.37
ATOM	819	C	PHE	A	913	49.216	52.291	21.331	1.00	21.37
ATOM	820	O	PHE	A	913	48.338	51.566	21.787	1.00	21.37
ATOM	821	CB	PHE	A	913	50.826	51.097	19.956	1.00	2.23
ATOM	822	CG	PHE	A	913	50.639	49.861	20.776	1.00	2.23
ATOM	823	CD1	PHE	A	913	50.389	48.681	20.185	1.00	2.23
ATOM	824	CD2	PHE	A	913	50.826	49.886	22.142	1.00	2.23
ATOM	825	CE1	PHE	A	913	50.330	47.610	20.870	1.00	2.23
ATOM	826	CE2	PHE	A	913	50.749	48.684	22.902	1.00	2.23
ATOM	827	CZ	PHE	A	913	50.503	47.593	22.238	1.00	2.23
ATOM	829	N	LEU	A	914	49.753	53.295	22.003	1.00	34.44
ATOM	830	CA	LEU	A	914	49.233	53.552	23.340	1.00	34.44
ATOM	831	C	LEU	A	914	47.770	54.028	23.202	1.00	34.44
ATOM	832	O	LEU	A	914	46.927	53.718	24.017	1.00	34.44

FIG. 6L

ATOM	833	CB	LEU	A	914	50.089	54.600	24.053	1.00	99.33
ATOM	834	CG	LEU	A	914	51.192	54.077	24.972	1.00	99.33
ATOM	835	CD1	LEU	A	914	52.365	55.032	24.979	1.00	99.33
ATOM	836	CD2	LEU	A	914	50.633	53.912	26.367	1.00	99.33
ATOM	838	N	ARG	A	915	47.489	54.720	22.111	1.00	38.92
ATOM	839	CA	ARG	A	915	46.202	55.332	21.795	1.00	38.92
ATOM	840	C	ARG	A	915	45.058	54.463	21.348	1.00	38.92
ATOM	841	O	ARG	A	915	43.891	54.728	21.700	1.00	38.92
ATOM	842	CB	ARG	A	915	46.422	56.347	20.720	1.00	6.43
ATOM	843	CG	ARG	A	915	46.646	57.788	21.276	1.00	6.43
ATOM	844	CD	ARG	A	915	47.992	58.402	21.097	1.00	6.43
ATOM	845	NE	ARG	A	915	48.094	59.491	22.107	1.00	6.43
ATOM	846	CZ	ARG	A	915	48.254	60.805	21.838	1.00	6.43
ATOM	847	NH1	ARG	A	915	48.331	61.314	20.610	1.00	6.43
ATOM	848	NH2	ARG	A	915	48.468	61.590	22.822	1.00	6.43
ATOM	855	N	LYS	A	916	45.399	53.475	20.520	1.00	22.32
ATOM	856	CA	LYS	A	916	44.513	52.462	20.007	1.00	22.32
ATOM	857	C	LYS	A	916	44.158	51.432	21.156	1.00	22.32
ATOM	858	O	LYS	A	916	43.680	50.278	20.864	1.00	22.32
ATOM	859	CB	LYS	A	916	45.275	51.740	18.908	1.00	23.97
ATOM	860	CG	LYS	A	916	46.735	51.281	19.327	1.00	23.97
ATOM	861	CD	LYS	A	916	46.899	50.099	20.472	1.00	23.97
ATOM	862	CE	LYS	A	916	46.886	48.726	19.880	1.00	23.97
ATOM	863	NZ	LYS	A	916	46.600	48.934	18.374	1.00	23.97
ATOM	868	N	SER	A	917	44.387	51.831	22.418	1.00	22.74
ATOM	869	CA	SER	A	917	44.179	51.001	23.600	1.00	22.74
ATOM	870	C	SER	A	917	43.034	51.499	24.516	1.00	22.74
ATOM	871	O	SER	A	917	42.627	50.829	25.545	1.00	22.74
ATOM	872	CB	SER	A	917	45.489	50.997	24.415	1.00	34.41
ATOM	873	OG	SER	A	917	45.310	50.676	25.795	1.00	34.41
ATOM	876	N	ARG	A	918	42.610	52.718	24.199	1.00	59.16
ATOM	877	CA	ARG	A	918	41.546	53.402	24.928	1.00	59.16
ATOM	878	C	ARG	A	918	40.240	52.937	24.293	1.00	59.16
ATOM	879	O	ARG	A	918	39.667	53.636	23.457	1.00	59.16
ATOM	880	CB	ARG	A	918	41.724	54.919	24.780	1.00	47.25
ATOM	881	CG	ARG	A	918	43.152	55.447	25.013	1.00	47.25
ATOM	882	CD	ARG	A	918	43.251	56.981	25.073	1.00	47.25
ATOM	883	NE	ARG	A	918	44.063	57.501	26.186	1.00	47.25
ATOM	884	CZ	ARG	A	918	44.349	58.794	26.368	1.00	47.25
ATOM	885	NH1	ARG	A	918	43.894	59.671	25.521	1.00	47.25
ATOM	886	NH2	ARG	A	918	45.092	59.226	27.374	1.00	47.25
ATOM	893	N	VAL	A	919	39.829	51.722	24.665	1.00	99.87
ATOM	894	CA	VAL	A	919	38.625	51.077	24.148	1.00	99.87
ATOM	895	C	VAL	A	919	37.442	52.049	24.208	1.00	99.87
ATOM	896	O	VAL	A	919	36.849	52.376	23.191	1.00	99.87
ATOM	897	CB	VAL	A	919	38.375	49.713	24.883	1.00	30.60
ATOM	898	CG1	VAL	A	919	39.007	48.626	24.110	1.00	30.60
ATOM	899	CG2	VAL	A	919	38.949	49.723	26.257	1.00	30.60
ATOM	901	N	LEU	A	920	37.111	52.497	25.405	1.00	36.31
ATOM	902	CA	LEU	A	920	36.115	53.513	25.648	1.00	36.31
ATOM	903	C	LEU	A	920	36.539	54.698	24.811	1.00	36.31
ATOM	904	O	LEU	A	920	37.065	55.646	25.312	1.00	36.31
ATOM	905	CB	LEU	A	920	36.201	53.928	27.088	1.00	11.95
ATOM	906	CG	LEU	A	920	34.951	54.248	27.902	1.00	11.95
ATOM	907	CD1	LEU	A	920	34.645	52.948	28.585	1.00	11.95
ATOM	908	CD2	LEU	A	920	35.117	55.350	28.954	1.00	11.95
ATOM	910	N	GLU	A	921	36.349	54.626	23.518	1.00	9.77

FIG. 6M

ATOM	911	CA	GLU	A	921	36.726	55.656	22.606	1.00	9.77
ATOM	912	C	GLU	A	921	36.937	54.877	21.314	1.00	9.77
ATOM	913	O	GLU	A	921	36.305	55.139	20.294	1.00	9.77
ATOM	914	CB	GLU	A	921	38.009	56.321	23.076	1.00	41.44
ATOM	915	CG	GLU	A	921	38.187	57.798	22.646	1.00	41.44
ATOM	916	CD	GLU	A	921	39.514	58.054	21.899	1.00	41.44
ATOM	917	OE1	GLU	A	921	40.583	58.228	22.581	1.00	41.44
ATOM	918	OE2	GLU	A	921	39.465	58.066	20.642	1.00	41.44
ATOM	920	N	THR	A	922	37.799	53.864	21.348	1.00	38.88
ATOM	921	CA	THR	A	922	38.110	53.051	20.167	1.00	38.88
ATOM	922	C	THR	A	922	36.981	52.136	19.842	1.00	38.88
ATOM	923	O	THR	A	922	36.505	52.013	18.726	1.00	38.88
ATOM	924	CB	THR	A	922	39.174	52.111	20.500	1.00	40.90
ATOM	925	OG1	THR	A	922	39.068	51.846	21.908	1.00	40.90
ATOM	926	CG2	THR	A	922	40.560	52.671	20.140	1.00	40.90
ATOM	929	N	ASP	A	923	36.604	51.443	20.897	1.00	29.76
ATOM	930	CA	ASP	A	923	35.585	50.420	20.901	1.00	29.76
ATOM	931	C	ASP	A	923	34.964	50.486	22.309	1.00	29.76
ATOM	932	O	ASP	A	923	35.466	49.896	23.271	1.00	29.76
ATOM	933	CB	ASP	A	923	36.294	49.081	20.662	1.00	100.00
ATOM	934	CG	ASP	A	923	35.357	47.934	20.521	1.00	100.00
ATOM	935	OD1	ASP	A	923	35.131	47.241	21.517	1.00	100.00
ATOM	936	OD2	ASP	A	923	34.854	47.713	19.413	1.00	100.00
ATOM	938	N	PRO	A	924	33.906	51.274	22.472	1.00	69.79
ATOM	939	CA	PRO	A	924	33.351	51.282	23.821	1.00	69.79
ATOM	940	C	PRO	A	924	32.633	49.968	24.194	1.00	69.79
ATOM	941	O	PRO	A	924	32.489	49.672	25.371	1.00	69.79
ATOM	942	CB	PRO	A	924	32.449	52.516	23.822	1.00	55.89
ATOM	943	CG	PRO	A	924	32.843	53.260	22.568	1.00	55.89
ATOM	944	CD	PRO	A	924	33.238	52.242	21.601	1.00	55.89
ATOM	945	N	ALA	A	925	32.206	49.183	23.199	1.00	100.00
ATOM	946	CA	ALA	A	925	31.555	47.887	23.453	1.00	100.00
ATOM	947	C	ALA	A	925	32.501	47.062	24.325	1.00	100.00
ATOM	948	O	ALA	A	925	32.137	46.651	25.428	1.00	100.00
ATOM	949	CB	ALA	A	925	31.278	47.156	22.146	1.00	100.00
ATOM	951	N	PHE	A	926	33.704	46.798	23.809	1.00	39.96
ATOM	952	CA	PHE	A	926	34.714	46.108	24.576	1.00	39.96
ATOM	953	C	PHE	A	926	34.808	46.862	25.859	1.00	39.96
ATOM	954	O	PHE	A	926	34.279	46.468	26.851	1.00	39.96
ATOM	955	CB	PHE	A	926	36.075	46.145	23.886	1.00	99.37
ATOM	956	CG	PHE	A	926	37.128	45.350	24.602	1.00	99.37
ATOM	957	CD1	PHE	A	926	37.270	43.990	24.365	1.00	99.37
ATOM	958	CD2	PHE	A	926	37.940	45.950	25.560	1.00	99.37
ATOM	959	CE1	PHE	A	926	38.192	43.248	25.071	1.00	99.37
ATOM	960	CE2	PHE	A	926	38.861	45.217	26.265	1.00	99.37
ATOM	961	CZ	PHE	A	926	38.987	43.863	26.023	1.00	99.37
ATOM	963	N	ALA	A	927	35.470	47.996	25.823	1.00	100.00
ATOM	964	CA	ALA	A	927	35.628	48.798	27.018	1.00	100.00
ATOM	965	C	ALA	A	927	34.627	48.539	28.167	1.00	100.00
ATOM	966	O	ALA	A	927	35.030	48.490	29.328	1.00	100.00
ATOM	967	CB	ALA	A	927	35.611	50.250	26.619	1.00	37.88
ATOM	969	N	ILE	A	928	33.343	48.348	27.845	1.00	71.50
ATOM	970	CA	ILE	A	928	32.287	48.137	28.866	1.00	71.50
ATOM	971	C	ILE	A	928	31.863	46.700	29.164	1.00	71.50
ATOM	972	O	ILE	A	928	31.579	46.352	30.301	1.00	71.50
ATOM	973	CB	ILE	A	928	30.987	48.939	28.510	1.00	96.87
ATOM	974	CG1	ILE	A	928	30.326	49.467	29.787	1.00	96.87

FIG. 6N,

ATOM	975	CG2	ILE	A	928	30.008	48.051	27.748	1.00	96.87
ATOM	976	CD1	ILE	A	928	28.888	49.846	29.624	1.00	96.87
ATOM	978	N	ALA	A	929	31.793	45.881	28.130	1.00	100.00
ATOM	979	CA	ALA	A	929	31.431	44.498	28.319	1.00	100.00
ATOM	980	C	ALA	A	929	32.550	43.917	29.163	1.00	100.00
ATOM	981	O	ALA	A	929	32.326	43.246	30.160	1.00	100.00
ATOM	982	CB	ALA	A	929	31.367	43.810	26.982	1.00	31.88
ATOM	984	N	ASN	A	930	33.767	44.220	28.737	1.00	37.33
ATOM	985	CA	ASN	A	930	35.009	43.775	29.380	1.00	37.33
ATOM	986	C	ASN	A	930	35.326	44.575	30.614	1.00	37.33
ATOM	987	O	ASN	A	930	36.020	44.110	31.496	1.00	37.33
ATOM	988	CB	ASN	A	930	36.163	43.843	28.378	1.00	87.25
ATOM	989	CG	ASN	A	930	36.469	42.497	27.753	1.00	87.25
ATOM	990	OD1	ASN	A	930	37.485	41.865	28.062	1.00	87.25
ATOM	991	ND2	ASN	A	930	35.590	42.051	26.865	1.00	87.25
ATOM	995	N	SER	A	931	34.828	45.807	30.629	1.00	35.86
ATOM	996	CA	SER	A	931	34.968	46.734	31.740	1.00	35.86
ATOM	997	C	SER	A	931	36.347	47.321	32.044	1.00	35.86
ATOM	998	O	SER	A	931	36.779	47.344	33.211	1.00	35.86
ATOM	999	CB	SER	A	931	34.413	46.039	32.992	1.00	47.04
ATOM	1000	OG	SER	A	931	34.049	44.700	32.650	1.00	47.04
ATOM	1003	N	THR	A	932	37.030	47.813	31.024	1.00	77.19
ATOM	1004	CA	THR	A	932	38.346	48.398	31.249	1.00	77.19
ATOM	1005	C	THR	A	932	38.655	49.585	30.346	1.00	77.19
ATOM	1006	O	THR	A	932	38.224	49.632	29.198	1.00	77.19
ATOM	1007	CB	THR	A	932	39.453	47.353	31.056	1.00	99.17
ATOM	1008	OG1	THR	A	932	39.813	47.299	29.676	1.00	99.17
ATOM	1009	CG2	THR	A	932	38.980	45.991	31.492	1.00	99.17
ATOM	1012	N	ALA	A	933	39.376	50.554	30.891	1.00	37.14
ATOM	1013	CA	ALA	A	933	39.814	51.734	30.120	1.00	37.14
ATOM	1014	C	ALA	A	933	40.655	51.286	28.911	1.00	37.14
ATOM	1015	O	ALA	A	933	40.255	51.495	27.792	1.00	37.14
ATOM	1016	CB	ALA	A	933	40.625	52.743	31.046	1.00	2.00
ATOM	1018	N	SER	A	934	41.814	50.674	29.139	1.00	18.52
ATOM	1019	CA	SER	A	934	42.656	50.117	28.038	1.00	18.52
ATOM	1020	C	SER	A	934	42.578	48.537	27.897	1.00	18.52
ATOM	1021	O	SER	A	934	42.047	47.842	28.815	1.00	18.52
ATOM	1022	CB	SER	A	934	44.114	50.415	28.347	1.00	25.65
ATOM	1023	OG	SER	A	934	44.983	49.645	27.568	1.00	25.65
ATOM	1026	N	THR	A	935	43.162	48.023	26.794	1.00	63.20
ATOM	1027	CA	THR	A	935	43.338	46.574	26.529	1.00	63.20
ATOM	1028	C	THR	A	935	44.762	46.121	26.957	1.00	63.20
ATOM	1029	O	THR	A	935	45.084	44.947	26.871	1.00	63.20
ATOM	1030	CB	THR	A	935	43.298	46.147	25.069	1.00	29.40
ATOM	1031	OG1	THR	A	935	44.470	46.603	24.393	1.00	29.40
ATOM	1032	CG2	THR	A	935	42.095	46.590	24.385	1.00	29.40
ATOM	1035	N	LEU	A	936	45.616	47.065	27.349	1.00	6.64
ATOM	1036	CA	LEU	A	936	46.959	46.811	27.861	1.00	6.64
ATOM	1037	C	LEU	A	936	46.654	46.775	29.277	1.00	6.64
ATOM	1038	O	LEU	A	936	45.478	46.916	29.572	1.00	6.64
ATOM	1039	CB	LEU	A	936	47.962	47.919	27.602	1.00	2.00
ATOM	1040	CG	LEU	A	936	48.129	48.224	26.129	1.00	2.00
ATOM	1041	CD1	LEU	A	936	48.725	49.731	25.993	1.00	2.00
ATOM	1042	CD2	LEU	A	936	48.953	47.147	25.523	1.00	2.00
ATOM	1044	N	SER	A	937	47.638	46.528	30.129	1.00	38.75
ATOM	1045	CA	SER	A	937	47.437	46.434	31.555	1.00	38.75
ATOM	1046	C	SER	A	937	48.615	47.041	32.342	1.00	38.75

FIG. 60

ATOM	1047	O	SER	A	937	49.664	47.405	31.785	1.00	38.75
ATOM	1048	CB	SER	A	937	47.257	44.979	31.954	1.00	80.09
ATOM	1049	OG	SER	A	937	48.471	44.274	31.851	1.00	80.09
ATOM	1052	N	SER	A	938	48.441	47.158	33.646	1.00	54.88
ATOM	1053	CA	SER	A	938	49.489	47.699	34.441	1.00	54.88
ATOM	1054	C	SER	A	938	50.807	47.155	33.941	1.00	54.88
ATOM	1055	O	SER	A	938	51.696	47.907	33.571	1.00	54.88
ATOM	1056	CB	SER	A	938	49.295	47.312	35.887	1.00	69.11
ATOM	1057	OG	SER	A	938	50.397	47.773	36.631	1.00	69.11
ATOM	1060	N	GLN	A	939	50.906	45.831	33.902	1.00	55.81
ATOM	1061	CA	GLN	A	939	52.106	45.148	33.492	1.00	55.81
ATOM	1062	C	GLN	A	939	52.644	45.445	32.132	1.00	55.81
ATOM	1063	O	GLN	A	939	53.750	45.896	32.027	1.00	55.81
ATOM	1064	CB	GLN	A	939	51.924	43.650	33.615	1.00	74.76
ATOM	1065	CG	GLN	A	939	52.012	43.126	35.014	1.00	74.76
ATOM	1066	CD	GLN	A	939	53.409	42.973	35.514	1.00	74.76
ATOM	1067	OE1	GLN	A	939	54.238	42.296	34.906	1.00	74.76
ATOM	1068	NE2	GLN	A	939	53.684	43.597	36.648	1.00	74.76
ATOM	1072	N	GLN	A	940	51.899	45.176	31.069	1.00	26.74
ATOM	1073	CA	GLN	A	940	52.446	45.439	29.736	1.00	26.74
ATOM	1074	C	GLN	A	940	52.963	46.884	29.791	1.00	26.74
ATOM	1075	O	GLN	A	940	53.929	47.302	29.115	1.00	26.74
ATOM	1076	CB	GLN	A	940	51.405	45.313	28.639	1.00	43.63
ATOM	1077	CG	GLN	A	940	51.815	46.080	27.393	1.00	43.63
ATOM	1078	CD	GLN	A	940	52.444	45.214	26.267	1.00	43.63
ATOM	1079	OE1	GLN	A	940	51.734	44.544	25.479	1.00	43.63
ATOM	1080	NE2	GLN	A	940	53.756	45.236	26.183	1.00	43.63
ATOM	1084	N	LEU	A	941	52.300	47.595	30.698	1.00	30.59
ATOM	1085	CA	LEU	A	941	52.514	48.989	30.932	1.00	30.59
ATOM	1086	C	LEU	A	941	53.800	49.234	31.599	1.00	30.59
ATOM	1087	O	LEU	A	941	54.611	49.971	31.068	1.00	30.59
ATOM	1088	CB	LEU	A	941	51.334	49.521	31.709	1.00	27.00
ATOM	1089	CG	LEU	A	941	50.344	50.390	30.959	1.00	27.00
ATOM	1090	CD1	LEU	A	941	50.253	51.655	31.777	1.00	27.00
ATOM	1091	CD2	LEU	A	941	50.770	50.642	29.576	1.00	27.00
ATOM	1093	N	LEU	A	942	53.992	48.683	32.768	1.00	26.63
ATOM	1094	CA	LEU	A	942	55.284	48.801	33.427	1.00	26.63
ATOM	1095	C	LEU	A	942	56.433	48.144	32.573	1.00	26.63
ATOM	1096	O	LEU	A	942	57.616	48.326	32.850	1.00	26.63
ATOM	1097	CB	LEU	A	942	55.208	48.083	34.741	1.00	3.59
ATOM	1098	CG	LEU	A	942	55.275	49.016	35.906	1.00	3.59
ATOM	1099	CD1	LEU	A	942	55.141	48.265	37.321	1.00	3.59
ATOM	1100	CD2	LEU	A	942	56.635	49.823	35.675	1.00	3.59
ATOM	1102	N	HIS	A	943	56.084	47.359	31.562	1.00	54.79
ATOM	1103	CA	HIS	A	943	57.101	46.756	30.741	1.00	54.79
ATOM	1104	C	HIS	A	943	57.531	47.932	29.905	1.00	54.79
ATOM	1105	O	HIS	A	943	58.389	48.665	30.324	1.00	54.79
ATOM	1106	CB	HIS	A	943	56.530	45.638	29.852	1.00	38.35
ATOM	1107	CG	HIS	A	943	56.799	44.246	30.345	1.00	38.35
ATOM	1108	ND1	HIS	A	943	56.846	43.914	31.682	1.00	38.35
ATOM	1109	CD2	HIS	A	943	56.988	43.092	29.671	1.00	38.35
ATOM	1110	CE1	HIS	A	943	57.050	42.619	31.812	1.00	38.35
ATOM	1111	NE2	HIS	A	943	57.143	42.096	30.603	1.00	38.35
ATOM	1115	N	PHE	A	944	56.905	48.115	28.741	1.00	4.19
ATOM	1116	CA	PHE	A	944	57.172	49.217	27.780	1.00	4.19
ATOM	1117	C	PHE	A	944	58.218	50.257	28.412	1.00	4.19
ATOM	1118	O	PHE	A	944	59.278	50.592	27.781	1.00	4.19

FIG. 6P

ATOM	1119	CB	PHE	A	944	55.878	49.913	27.509	1.00	28.23
ATOM	1120	CG	PHE	A	944	55.036	49.255	26.489	1.00	28.23
ATOM	1121	CD1	PHE	A	944	53.632	49.319	26.610	1.00	28.23
ATOM	1122	CD2	PHE	A	944	55.605	48.780	25.336	1.00	28.23
ATOM	1123	CE1	PHE	A	944	52.813	48.958	25.614	1.00	28.23
ATOM	1124	CE2	PHE	A	944	54.769	48.399	24.289	1.00	28.23
ATOM	1125	CZ	PHE	A	944	53.342	48.504	24.452	1.00	28.23
ATOM	1127	N	ALA	A	945	57.874	50.702	29.637	1.00	24.23
ATOM	1128	CA	ALA	A	945	58.742	51.520	30.434	1.00	24.23
ATOM	1129	C	ALA	A	945	59.943	50.648	30.375	1.00	24.23
ATOM	1130	O	ALA	A	945	60.623	50.707	29.408	1.00	24.23
ATOM	1131	CB	ALA	A	945	58.270	51.631	31.839	1.00	16.89
ATOM	1133	N	ALA	A	946	60.153	49.775	31.366	1.00	23.93
ATOM	1134	CA	ALA	A	946	61.327	48.819	31.493	1.00	23.93
ATOM	1135	C	ALA	A	946	62.279	48.525	30.320	1.00	23.93
ATOM	1136	O	ALA	A	946	63.460	48.674	30.432	1.00	23.93
ATOM	1137	CB	ALA	A	946	60.834	47.495	32.054	1.00	76.24
ATOM	1139	N	ASP	A	947	61.796	48.078	29.188	1.00	9.63
ATOM	1140	CA	ASP	A	947	62.727	47.858	28.131	1.00	9.63
ATOM	1141	C	ASP	A	947	63.169	49.132	27.456	1.00	9.63
ATOM	1142	O	ASP	A	947	63.604	49.093	26.290	1.00	9.63
ATOM	1143	CB	ASP	A	947	62.145	46.880	27.114	1.00	90.89
ATOM	1144	CG	ASP	A	947	61.065	47.493	26.259	1.00	90.89
ATOM	1145	OD1	ASP	A	947	60.143	46.747	25.854	1.00	90.89
ATOM	1146	OD2	ASP	A	947	61.128	48.707	25.978	1.00	90.89
ATOM	1148	N	VAL	A	948	63.024	50.287	28.098	1.00	60.29
ATOM	1149	CA	VAL	A	948	63.435	51.532	27.459	1.00	60.29
ATOM	1150	C	VAL	A	948	64.572	51.963	28.376	1.00	60.29
ATOM	1151	O	VAL	A	948	65.604	52.405	27.907	1.00	60.29
ATOM	1152	CB	VAL	A	948	62.213	52.606	27.324	1.00	2.00
ATOM	1153	CG1	VAL	A	948	62.752	54.133	26.901	1.00	2.00
ATOM	1154	CG2	VAL	A	948	61.348	52.297	26.209	1.00	2.00
ATOM	1156	N	ALA	A	949	64.402	51.773	29.686	1.00	12.91
ATOM	1157	CA	ALA	A	949	65.448	52.097	30.677	1.00	12.91
ATOM	1158	C	ALA	A	949	66.681	51.382	30.188	1.00	12.91
ATOM	1159	O	ALA	A	949	67.733	52.000	29.956	1.00	12.91
ATOM	1160	CB	ALA	A	949	65.135	51.617	32.017	1.00	2.00
ATOM	1162	N	ARG	A	950	66.484	50.078	30.000	1.00	22.64
ATOM	1163	CA	ARG	A	950	67.422	49.105	29.537	1.00	22.64
ATOM	1164	C	ARG	A	950	68.106	49.588	28.340	1.00	22.64
ATOM	1165	O	ARG	A	950	69.275	49.681	28.386	1.00	22.64
ATOM	1166	CB	ARG	A	950	66.702	47.783	29.233	1.00	87.27
ATOM	1167	CG	ARG	A	950	67.146	46.606	30.102	1.00	87.27
ATOM	1168	CD	ARG	A	950	66.806	45.233	29.493	1.00	87.27
ATOM	1169	NE	ARG	A	950	65.466	45.208	28.912	1.00	87.27
ATOM	1170	CZ	ARG	A	950	64.341	44.977	29.580	1.00	87.27
ATOM	1171	NH1	ARG	A	950	64.357	44.746	30.879	1.00	87.27
ATOM	1172	NH2	ARG	A	950	63.188	45.019	28.941	1.00	87.27
ATOM	1179	N	GLY	A	951	67.435	49.846	27.241	1.00	33.31
ATOM	1180	CA	GLY	A	951	68.177	50.360	26.102	1.00	33.31
ATOM	1181	C	GLY	A	951	68.720	51.768	26.462	1.00	33.31
ATOM	1182	O	GLY	A	951	69.514	52.379	25.745	1.00	33.31
ATOM	1184	N	MET	A	952	68.277	52.318	27.588	1.00	48.02
ATOM	1185	CA	MET	A	952	68.774	53.615	27.949	1.00	48.02
ATOM	1186	C	MET	A	952	70.030	53.440	28.759	1.00	48.02
ATOM	1187	O	MET	A	952	70.861	54.316	28.719	1.00	48.02
ATOM	1188	CB	MET	A	952	67.721	54.442	28.720	1.00	58.75

ATOM	1189	CG	MET	A	952	67.277	55.792	28.089	1.00	58.75
ATOM	1190	SD	MET	A	952	67.797	56.265	26.390	1.00	58.75
ATOM	1191	CE	MET	A	952	69.079	57.471	26.826	1.00	58.75
ATOM	1193	N	ASP	A	953	70.145	52.325	29.494	1.00	30.83
ATOM	1194	CA	ASP	A	953	71.299	51.942	30.317	1.00	30.83
ATOM	1195	C	ASP	A	953	72.393	51.689	29.346	1.00	30.83
ATOM	1196	O	ASP	A	953	73.521	52.078	29.523	1.00	30.83
ATOM	1197	CB	ASP	A	953	71.084	50.617	30.955	1.00	30.69
ATOM	1198	CG	ASP	A	953	71.512	50.589	32.381	1.00	30.69
ATOM	1199	OD1	ASP	A	953	71.504	51.661	32.997	1.00	30.69
ATOM	1200	OD2	ASP	A	953	71.838	49.485	32.907	1.00	30.69
ATOM	1202	N	TYR	A	954	72.031	50.999	28.292	1.00	19.34
ATOM	1203	CA	TYR	A	954	72.952	50.630	27.239	1.00	19.34
ATOM	1204	C	TYR	A	954	73.559	51.896	26.762	1.00	19.34
ATOM	1205	O	TYR	A	954	74.529	52.327	27.362	1.00	19.34
ATOM	1206	CB	TYR	A	954	72.236	49.887	26.117	1.00	37.26
ATOM	1207	CG	TYR	A	954	73.181	49.115	25.244	1.00	37.26
ATOM	1208	CD1	TYR	A	954	74.158	48.238	25.784	1.00	37.26
ATOM	1209	CD2	TYR	A	954	73.149	49.300	23.871	1.00	37.26
ATOM	1210	CE1	TYR	A	954	75.072	47.594	24.942	1.00	37.26
ATOM	1211	CE2	TYR	A	954	74.042	48.676	23.041	1.00	37.26
ATOM	1212	CZ	TYR	A	954	74.993	47.843	23.568	1.00	37.26
ATOM	1213	OH	TYR	A	954	75.859	47.367	22.645	1.00	37.26
ATOM	1216	N	LEU	A	955	72.967	52.501	25.722	1.00	49.71
ATOM	1217	CA	LEU	A	955	73.404	53.781	25.150	1.00	49.71
ATOM	1218	C	LEU	A	955	73.854	54.641	26.293	1.00	49.71
ATOM	1219	O	LEU	A	955	74.950	55.109	26.279	1.00	49.71
ATOM	1220	CB	LEU	A	955	72.272	54.530	24.439	1.00	17.74
ATOM	1221	CG	LEU	A	955	71.456	53.937	23.292	1.00	17.74
ATOM	1222	CD1	LEU	A	955	69.972	54.493	23.397	1.00	17.74
ATOM	1223	CD2	LEU	A	955	71.989	54.345	21.914	1.00	17.74
ATOM	1225	N	SER	A	956	73.012	54.840	27.293	1.00	34.64
ATOM	1226	CA	SER	A	956	73.430	55.663	28.404	1.00	34.64
ATOM	1227	C	SER	A	956	74.843	55.360	28.778	1.00	34.64
ATOM	1228	O	SER	A	956	75.701	56.218	28.579	1.00	34.64
ATOM	1229	CB	SER	A	956	72.561	55.495	29.622	1.00	37.38
ATOM	1230	OG	SER	A	956	73.071	56.228	30.699	1.00	37.38
ATOM	1233	N	GLN	A	957	75.134	54.188	29.321	1.00	33.59
ATOM	1234	CA	GLN	A	957	76.511	53.895	29.680	1.00	33.59
ATOM	1235	C	GLN	A	957	77.379	53.837	28.410	1.00	33.59
ATOM	1236	O	GLN	A	957	77.719	52.798	27.943	1.00	33.59
ATOM	1237	CB	GLN	A	957	76.583	52.568	30.455	1.00	42.10
ATOM	1238	CG	GLN	A	957	76.621	52.721	32.002	1.00	42.10
ATOM	1239	CD	GLN	A	957	77.483	53.951	32.500	1.00	42.10
ATOM	1240	OE1	GLN	A	957	78.321	54.499	31.739	1.00	42.10
ATOM	1241	NE2	GLN	A	957	77.274	54.367	33.780	1.00	42.10
ATOM	1245	N	LYS	A	958	77.739	54.952	27.823	1.00	99.18
ATOM	1246	CA	LYS	A	958	78.543	54.854	26.620	1.00	99.18
ATOM	1247	C	LYS	A	958	78.688	56.227	26.039	1.00	99.18
ATOM	1248	O	LYS	A	958	79.111	56.370	24.897	1.00	99.18
ATOM	1249	CB	LYS	A	958	77.880	53.934	25.586	1.00	99.74
ATOM	1250	CG	LYS	A	958	78.545	52.582	25.404	1.00	99.74
ATOM	1251	CD	LYS	A	958	77.830	51.738	24.360	1.00	99.74
ATOM	1252	CE	LYS	A	958	77.997	50.238	24.629	1.00	99.74
ATOM	1253	NZ	LYS	A	958	78.459	49.456	23.434	1.00	99.74
ATOM	1258	N	GLN	A	959	78.327	57.233	26.832	1.00	73.45
ATOM	1259	CA	GLN	A	959	78.423	58.615	26.402	1.00	73.45

FIG. 6R

ATOM	1260	C	GLN	A	959	77.378	58.947	25.376	1.00	73.45
ATOM	1261	O	GLN	A	959	77.493	59.970	24.702	1.00	73.45
ATOM	1262	CB	GLN	A	959	79.785	58.882	25.784	1.00	19.35
ATOM	1263	CG	GLN	A	959	80.899	58.069	26.399	1.00	19.35
ATOM	1264	CD	GLN	A	959	80.957	58.449	27.805	1.00	19.35
ATOM	1265	OE1	GLN	A	959	80.252	59.453	28.221	1.00	19.35
ATOM	1266	NE2	GLN	A	959	81.763	57.708	28.610	1.00	19.35
ATOM	1270	N	PHE	A	960	76.376	58.075	25.242	1.00	36.08
ATOM	1271	CA	PHE	A	960	75.312	58.292	24.262	1.00	36.08
ATOM	1272	C	PHE	A	960	74.223	59.102	24.956	1.00	36.08
ATOM	1273	O	PHE	A	960	73.754	58.762	26.078	1.00	36.08
ATOM	1274	CB	PHE	A	960	74.810	56.957	23.718	1.00	85.11
ATOM	1275	CG	PHE	A	960	75.670	56.407	22.614	1.00	85.11
ATOM	1276	CD1	PHE	A	960	76.531	55.349	22.839	1.00	85.11
ATOM	1277	CD2	PHE	A	960	75.656	56.981	21.350	1.00	85.11
ATOM	1278	CE1	PHE	A	960	77.361	54.879	21.822	1.00	85.11
ATOM	1279	CE2	PHE	A	960	76.493	56.505	20.330	1.00	85.11
ATOM	1280	CZ	PHE	A	960	77.338	55.461	20.572	1.00	85.11
ATOM	1282	N	ILE	A	961	73.918	60.227	24.300	1.00	30.22
ATOM	1283	CA	ILE	A	961	72.939	61.196	24.749	1.00	30.22
ATOM	1284	C	ILE	A	961	71.858	61.213	23.713	1.00	30.22
ATOM	1285	O	ILE	A	961	72.112	61.420	22.545	1.00	30.22
ATOM	1286	CB	ILE	A	961	73.536	62.578	24.911	1.00	71.39
ATOM	1287	CG1	ILE	A	961	74.693	62.526	25.899	1.00	71.39
ATOM	1288	CG2	ILE	A	961	72.488	63.518	25.442	1.00	71.39
ATOM	1289	CD1	ILE	A	961	75.888	63.302	25.476	1.00	71.39
ATOM	1291	N	HIS	A	962	70.627	61.034	24.158	1.00	80.58
ATOM	1292	CA	HIS	A	962	69.524	60.924	23.236	1.00	80.58
ATOM	1293	C	HIS	A	962	68.798	62.196	22.692	1.00	80.58
ATOM	1294	O	HIS	A	962	69.179	62.676	21.629	1.00	80.58
ATOM	1295	CB	HIS	A	962	68.584	59.904	23.855	1.00	39.42
ATOM	1296	CG	HIS	A	962	67.415	59.585	23.008	1.00	39.42
ATOM	1297	ND1	HIS	A	962	67.142	58.316	22.575	1.00	39.42
ATOM	1298	CD2	HIS	A	962	66.450	60.378	22.499	1.00	39.42
ATOM	1299	CE1	HIS	A	962	66.052	58.335	21.832	1.00	39.42
ATOM	1300	NE2	HIS	A	962	65.617	59.580	21.772	1.00	39.42
ATOM	1304	N	ARG	A	963	67.745	62.694	23.367	1.00	25.62
ATOM	1305	CA	ARG	A	963	67.008	63.920	22.979	1.00	25.62
ATOM	1306	C	ARG	A	963	65.777	63.852	22.084	1.00	25.62
ATOM	1307	O	ARG	A	963	65.762	64.331	20.941	1.00	25.62
ATOM	1308	CB	ARG	A	963	67.977	64.955	22.380	1.00	98.75
ATOM	1309	CG	ARG	A	963	69.318	65.061	23.081	1.00	98.75
ATOM	1310	CD	ARG	A	963	70.230	66.016	22.356	1.00	98.75
ATOM	1311	NE	ARG	A	963	70.718	65.501	21.087	1.00	98.75
ATOM	1312	CZ	ARG	A	963	70.212	65.832	19.911	1.00	98.75
ATOM	1313	NH1	ARG	A	963	69.200	66.680	19.852	1.00	98.75
ATOM	1314	NH2	ARG	A	963	70.717	65.321	18.801	1.00	98.75
ATOM	1321	N	ASN	A	964	64.738	63.276	22.661	1.00	47.91
ATOM	1322	CA	ASN	A	964	63.442	63.070	22.035	1.00	47.91
ATOM	1323	C	ASN	A	964	63.235	61.618	22.246	1.00	47.91
ATOM	1324	O	ASN	A	964	63.068	60.856	21.302	1.00	47.91
ATOM	1325	CB	ASN	A	964	63.453	63.377	20.538	1.00	84.77
ATOM	1326	CG	ASN	A	964	62.453	64.459	20.153	1.00	84.77
ATOM	1327	OD1	ASN	A	964	61.509	64.768	20.902	1.00	84.77
ATOM	1328	ND2	ASN	A	964	62.653	65.039	18.977	1.00	84.77
ATOM	1332	N	LEU	A	965	63.366	61.249	23.509	1.00	96.70
ATOM	1333	CA	LEU	A	965	63.148	59.897	23.937	1.00	96.70

FIG. 6S

ATOM	1334	C	LEU	A	965	61.836	60.220	24.659	1.00	96.70
ATOM	1335	O	LEU	A	965	61.784	60.527	25.833	1.00	96.70
ATOM	1336	CB	LEU	A	965	64.352	59.382	24.805	1.00	17.46
ATOM	1337	CG	LEU	A	965	64.456	58.589	26.099	1.00	17.46
ATOM	1338	CD1	LEU	A	965	65.774	58.784	26.891	1.00	17.46
ATOM	1339	CD2	LEU	A	965	63.423	59.114	26.967	1.00	17.46
ATOM	1341	N	ALA	A	966	60.794	60.283	23.833	1.00	71.46
ATOM	1342	CA	ALA	A	966	59.408	60.534	24.219	1.00	71.46
ATOM	1343	C	ALA	A	966	58.601	59.518	23.395	1.00	71.46
ATOM	1344	O	ALA	A	966	59.009	59.122	22.314	1.00	71.46
ATOM	1345	CB	ALA	A	966	59.005	61.933	23.885	1.00	62.29
ATOM	1347	N	ALA	A	967	57.457	59.105	23.908	1.00	34.40
ATOM	1348	CA	ALA	A	967	56.641	58.086	23.249	1.00	34.40
ATOM	1349	C	ALA	A	967	56.585	58.066	21.726	1.00	34.40
ATOM	1350	O	ALA	A	967	56.689	57.011	21.106	1.00	34.40
ATOM	1351	CB	ALA	A	967	55.236	58.088	23.807	1.00	31.96
ATOM	1353	N	ARG	A	968	56.462	59.208	21.094	1.00	9.59
ATOM	1354	CA	ARG	A	968	56.309	59.113	19.678	1.00	9.59
ATOM	1355	C	ARG	A	968	57.467	58.532	19.054	1.00	9.59
ATOM	1356	O	ARG	A	968	57.335	58.106	17.930	1.00	9.59
ATOM	1357	CB	ARG	A	968	55.960	60.480	19.013	1.00	12.36
ATOM	1358	CG	ARG	A	968	56.480	61.806	19.751	1.00	12.36
ATOM	1359	CD	ARG	A	968	56.426	62.907	18.727	1.00	12.36
ATOM	1360	NE	ARG	A	968	57.453	63.898	18.879	1.00	12.36
ATOM	1361	CZ	ARG	A	968	57.608	64.568	19.994	1.00	12.36
ATOM	1362	NH1	ARG	A	968	56.746	64.307	20.994	1.00	12.36
ATOM	1363	NH2	ARG	A	968	58.718	65.297	20.206	1.00	12.36
ATOM	1370	N	ASN	A	969	58.611	58.550	19.735	1.00	56.22
ATOM	1371	CA	ASN	A	969	59.878	58.043	19.179	1.00	56.22
ATOM	1372	C	ASN	A	969	60.309	56.672	19.730	1.00	56.22
ATOM	1373	O	ASN	A	969	61.472	56.327	19.673	1.00	56.22
ATOM	1374	CB	ASN	A	969	61.011	59.053	19.444	1.00	99.68
ATOM	1375	CG	ASN	A	969	60.674	60.482	18.998	1.00	99.68
ATOM	1376	OD1	ASN	A	969	60.213	61.303	19.787	1.00	99.68
ATOM	1377	ND2	ASN	A	969	60.926	60.780	17.732	1.00	99.68
ATOM	1381	N	ILE	A	970	59.351	55.935	20.288	1.00	10.68
ATOM	1382	CA	ILE	A	970	59.507	54.683	20.853	1.00	10.68
ATOM	1383	C	ILE	A	970	58.651	53.708	20.079	1.00	10.68
ATOM	1384	O	ILE	A	970	57.450	53.865	20.060	1.00	10.68
ATOM	1385	CB	ILE	A	970	59.003	54.602	22.158	1.00	11.62
ATOM	1386	CG1	ILE	A	970	59.808	55.496	23.084	1.00	11.62
ATOM	1387	CG2	ILE	A	970	59.191	53.056	22.620	1.00	11.62
ATOM	1388	CD1	ILE	A	970	61.263	55.730	22.600	1.00	11.62
ATOM	1390	N	LEU	A	971	59.250	52.676	19.496	1.00	31.69
ATOM	1391	CA	LEU	A	971	58.518	51.699	18.733	1.00	31.69
ATOM	1392	C	LEU	A	971	58.148	50.357	19.369	1.00	31.69
ATOM	1393	O	LEU	A	971	58.938	49.792	20.148	1.00	31.69
ATOM	1394	CB	LEU	A	971	59.308	51.333	17.535	1.00	17.23
ATOM	1395	CG	LEU	A	971	59.702	52.411	16.632	1.00	17.23
ATOM	1396	CD1	LEU	A	971	60.981	51.973	16.005	1.00	17.23
ATOM	1397	CD2	LEU	A	971	58.629	52.642	15.646	1.00	17.23
ATOM	1399	N	VAL	A	972	56.953	49.832	19.017	1.00	20.91
ATOM	1400	CA	VAL	A	972	56.655	48.486	19.475	1.00	20.91
ATOM	1401	C	VAL	A	972	56.862	47.491	18.389	1.00	20.91
ATOM	1402	O	VAL	A	972	56.022	47.375	17.523	1.00	20.91
ATOM	1403	CB	VAL	A	972	55.344	48.349	19.953	1.00	9.13
ATOM	1404	CG1	VAL	A	972	55.362	47.291	21.081	1.00	9.13

FIG. 6T

ATOM	1405	CG2	VAL	A	972	54.797	49.894	20.467	1.00	9.13
ATOM	1407	N	GLY	A	973	58.077	46.873	18.414	1.00	32.46
ATOM	1408	CA	GLY	A	973	58.514	45.851	17.466	1.00	32.46
ATOM	1409	C	GLY	A	973	58.012	44.434	17.814	1.00	32.46
ATOM	1410	O	GLY	A	973	57.324	44.254	18.816	1.00	32.46
ATOM	1412	N	GLU	A	974	58.393	43.403	17.055	1.00	22.44
ATOM	1413	CA	GLU	A	974	57.846	42.109	17.351	1.00	22.44
ATOM	1414	C	GLU	A	974	57.902	41.725	18.793	1.00	22.44
ATOM	1415	O	GLU	A	974	58.809	42.041	19.510	1.00	22.44
ATOM	1416	CB	GLU	A	974	58.364	41.035	16.394	1.00	65.78
ATOM	1417	CG	GLU	A	974	57.385	40.798	15.138	1.00	65.78
ATOM	1418	CD	GLU	A	974	55.821	40.585	15.469	1.00	65.78
ATOM	1419	OE1	GLU	A	974	55.398	40.463	16.656	1.00	65.78
ATOM	1420	OE2	GLU	A	974	55.005	40.540	14.512	1.00	65.78
ATOM	1422	N	ASN	A	975	56.767	41.210	19.246	1.00	22.08
ATOM	1423	CA	ASN	A	975	56.540	40.717	20.627	1.00	22.08
ATOM	1424	C	ASN	A	975	56.037	41.756	21.638	1.00	22.08
ATOM	1425	O	ASN	A	975	55.968	41.482	22.844	1.00	22.08
ATOM	1426	CB	ASN	A	975	57.810	40.016	21.140	1.00	99.25
ATOM	1427	CG	ASN	A	975	58.074	38.679	20.438	1.00	99.25
ATOM	1428	OD1	ASN	A	975	58.836	37.859	20.929	1.00	99.25
ATOM	1429	ND2	ASN	A	975	57.446	38.465	19.292	1.00	99.25
ATOM	1433	N	TYR	A	976	55.656	42.932	21.134	1.00	30.29
ATOM	1434	CA	TYR	A	976	55.204	44.013	21.972	1.00	30.29
ATOM	1435	C	TYR	A	976	56.427	44.631	22.697	1.00	30.29
ATOM	1436	O	TYR	A	976	56.331	45.214	23.759	1.00	30.29
ATOM	1437	CB	TYR	A	976	54.157	43.463	22.893	1.00	71.60
ATOM	1438	CG	TYR	A	976	53.001	42.961	22.089	1.00	71.60
ATOM	1439	CD1	TYR	A	976	52.698	41.611	22.036	1.00	71.60
ATOM	1440	CD2	TYR	A	976	52.229	43.840	21.339	1.00	71.60
ATOM	1441	CE1	TYR	A	976	51.652	41.145	21.243	1.00	71.60
ATOM	1442	CE2	TYR	A	976	51.181	43.390	20.547	1.00	71.60
ATOM	1443	CZ	TYR	A	976	50.895	42.043	20.491	1.00	71.60
ATOM	1444	OH	TYR	A	976	49.905	41.588	19.655	1.00	71.60
ATOM	1447	N	VAL	A	977	57.569	44.513	22.047	1.00	35.58
ATOM	1448	CA	VAL	A	977	58.837	44.988	22.597	1.00	35.58
ATOM	1449	C	VAL	A	977	59.247	46.367	22.101	1.00	35.58
ATOM	1450	O	VAL	A	977	59.495	46.616	20.903	1.00	35.58
ATOM	1451	CB	VAL	A	977	59.994	43.975	22.316	1.00	54.29
ATOM	1452	CG1	VAL	A	977	61.110	44.134	23.340	1.00	54.29
ATOM	1453	CG2	VAL	A	977	59.418	42.533	22.339	1.00	54.29
ATOM	1455	N	ALA	A	978	59.355	47.233	23.082	1.00	36.83
ATOM	1456	CA	ALA	A	978	59.628	48.594	22.857	1.00	36.83
ATOM	1457	C	ALA	A	978	61.086	49.005	22.550	1.00	36.83
ATOM	1458	O	ALA	A	978	61.937	48.823	23.380	1.00	36.83
ATOM	1459	CB	ALA	A	978	59.142	49.265	24.019	1.00	27.14
ATOM	1461	N	LYS	A	979	61.368	49.570	21.374	1.00	42.93
ATOM	1462	CA	LYS	A	979	62.704	50.023	21.063	1.00	42.93
ATOM	1463	C	LYS	A	979	63.002	51.530	20.907	1.00	42.93
ATOM	1464	O	LYS	A	979	62.175	52.352	20.414	1.00	42.93
ATOM	1465	CB	LYS	A	979	63.190	49.433	19.798	1.00	32.23
ATOM	1466	CG	LYS	A	979	62.273	48.708	19.039	1.00	32.23
ATOM	1467	CD	LYS	A	979	62.556	47.230	19.416	1.00	32.23
ATOM	1468	CE	LYS	A	979	63.156	46.356	18.275	1.00	32.23
ATOM	1469	NZ	LYS	A	979	63.744	45.144	18.883	1.00	32.23
ATOM	1474	N	ILE	A	980	64.233	51.887	21.275	1.00	2.00
ATOM	1475	CA	ILE	A	980	64.639	53.265	21.099	1.00	2.00

FIG. 6U

ATOM	1476	C	ILE	A	980	65.044	53.446	19.649	1.00	2.00
ATOM	1477	O	ILE	A	980	65.191	52.445	18.913	1.00	2.00
ATOM	1478	CB	ILE	A	980	65.717	53.649	22.013	1.00	22.25
ATOM	1479	CG1	ILE	A	980	65.318	53.372	23.463	1.00	22.25
ATOM	1480	CG2	ILE	A	980	65.839	55.073	21.885	1.00	22.25
ATOM	1481	CD1	ILE	A	980	66.358	53.040	24.467	1.00	22.25
ATOM	1483	N	ALA	A	981	65.129	54.715	19.235	1.00	37.10
ATOM	1484	CA	ALA	A	981	65.489	55.166	17.870	1.00	37.10
ATOM	1485	C	ALA	A	981	65.426	56.684	17.652	1.00	37.10
ATOM	1486	O	ALA	A	981	64.905	57.454	18.494	1.00	37.10
ATOM	1487	CB	ALA	A	981	64.634	54.620	16.964	1.00	12.10
ATOM	1489	N	ASP	A	982	65.933	57.120	16.508	1.00	81.89
ATOM	1490	CA	ASP	A	982	65.907	58.525	16.186	1.00	81.89
ATOM	1491	C	ASP	A	982	66.821	59.190	17.201	1.00	81.89
ATOM	1492	O	ASP	A	982	66.877	60.416	17.342	1.00	81.89
ATOM	1493	CB	ASP	A	982	64.465	59.029	16.284	1.00	22.36
ATOM	1494	CG	ASP	A	982	64.352	60.357	16.999	1.00	22.36
ATOM	1495	OD1	ASP	A	982	64.517	61.390	16.281	1.00	22.36
ATOM	1496	OD2	ASP	A	982	64.112	60.353	18.252	1.00	22.36
ATOM	1498	N	PHE	A	983	67.540	58.353	17.922	1.00	90.03
ATOM	1499	CA	PHE	A	983	68.502	58.819	18.897	1.00	90.03
ATOM	1500	C	PHE	A	983	69.521	59.638	18.083	1.00	90.03
ATOM	1501	O	PHE	A	983	69.436	59.728	16.844	1.00	90.03
ATOM	1502	CB	PHE	A	983	69.205	57.599	19.489	1.00	100.00
ATOM	1503	CG	PHE	A	983	69.417	56.489	18.475	1.00	100.00
ATOM	1504	CD1	PHE	A	983	70.419	56.593	17.502	1.00	100.00
ATOM	1505	CD2	PHE	A	983	68.567	55.387	18.435	1.00	100.00
ATOM	1506	CE1	PHE	A	983	70.557	55.624	16.513	1.00	100.00
ATOM	1507	CE2	PHE	A	983	68.704	54.418	17.449	1.00	100.00
ATOM	1508	CZ	PHE	A	983	69.698	54.537	16.488	1.00	100.00
ATOM	1510	N	GLY	A	984	70.493	60.226	18.770	1.00	59.78
ATOM	1511	CA	GLY	A	984	71.533	60.957	18.060	1.00	59.78
ATOM	1512	C	GLY	A	984	72.821	60.159	18.193	1.00	59.78
ATOM	1513	O	GLY	A	984	72.900	59.221	19.019	1.00	59.78
ATOM	1515	N	LEU	A	985	73.816	60.488	17.379	1.00	99.32
ATOM	1516	CA	LEU	A	985	75.094	59.791	17.454	1.00	99.32
ATOM	1517	C	LEU	A	985	75.886	60.603	18.440	1.00	99.32
ATOM	1518	O	LEU	A	985	77.068	60.348	18.669	1.00	99.32
ATOM	1519	CB	LEU	A	985	75.824	59.786	16.106	1.00	100.00
ATOM	1520	CG	LEU	A	985	75.453	58.753	15.036	1.00	100.00
ATOM	1521	CD1	LEU	A	985	74.707	57.590	15.651	1.00	100.00
ATOM	1522	CD2	LEU	A	985	74.604	59.428	13.971	1.00	100.00
ATOM	1524	N	SER	A	986	75.211	61.587	19.020	1.00	37.75
ATOM	1525	CA	SER	A	986	75.828	62.476	19.989	1.00	37.75
ATOM	1526	C	SER	A	986	76.413	61.806	21.210	1.00	37.75
ATOM	1527	O	SER	A	986	75.708	61.541	22.143	1.00	37.75
ATOM	1528	CB	SER	A	986	74.830	63.525	20.445	1.00	99.91
ATOM	1529	OG	SER	A	986	75.198	64.776	19.917	1.00	99.91
ATOM	1532	N	ARG	A	987	77.710	61.513	21.216	1.00	63.13
ATOM	1533	CA	ARG	A	987	78.285	60.910	22.407	1.00	63.13
ATOM	1534	C	ARG	A	987	79.243	61.904	22.979	1.00	63.13
ATOM	1535	O	ARG	A	987	80.058	62.476	22.270	1.00	63.13
ATOM	1536	CB	ARG	A	987	78.964	59.567	22.132	1.00	87.40
ATOM	1537	CG	ARG	A	987	79.870	59.529	20.947	1.00	87.40
ATOM	1538	CD	ARG	A	987	81.110	58.722	21.273	1.00	87.40
ATOM	1539	NE	ARG	A	987	80.807	57.654	22.217	1.00	87.40
ATOM	1540	CZ	ARG	A	987	80.782	56.366	21.898	1.00	87.40

FIG. 6V

ATOM	1541	NH1	ARG	A	987	81.042	55.981	20.658	1.00	87.40
ATOM	1542	NH2	ARG	A	987	80.506	55.463	22.824	1.00	87.40
ATOM	1549	N	GLY	A	988	79.090	62.096	24.282	1.00	28.62
ATOM	1550	CA	GLY	A	988	79.833	63.044	25.072	1.00	28.62
ATOM	1551	C	GLY	A	988	79.268	63.073	26.476	1.00	28.62
ATOM	1552	O	GLY	A	988	78.558	62.156	26.816	1.00	28.62
ATOM	1554	N	GLN	A	989	79.612	64.094	27.270	1.00	22.70
ATOM	1555	CA	GLN	A	989	79.214	64.322	28.682	1.00	22.70
ATOM	1556	C	GLN	A	989	78.188	65.518	28.775	1.00	22.70
ATOM	1557	O	GLN	A	989	77.534	65.676	29.785	1.00	22.70
ATOM	1558	CB	GLN	A	989	80.449	64.647	29.536	1.00	98.73
ATOM	1559	CG	GLN	A	989	80.240	64.572	31.049	1.00	98.73
ATOM	1560	CD	GLN	A	989	81.127	65.539	31.844	1.00	98.73
ATOM	1561	OE1	GLN	A	989	81.240	66.712	31.510	1.00	98.73
ATOM	1562	NE2	GLN	A	989	81.746	65.043	32.901	1.00	98.73
ATOM	1566	N	GLU	A	990	78.055	66.323	27.724	1.00	47.13
ATOM	1567	CA	GLU	A	990	77.173	67.478	27.725	1.00	47.13
ATOM	1568	C	GLU	A	990	77.106	67.842	26.251	1.00	47.13
ATOM	1569	O	GLU	A	990	78.116	67.765	25.565	1.00	47.13
ATOM	1570	CB	GLU	A	990	77.830	68.612	28.534	1.00	77.23
ATOM	1571	CG	GLU	A	990	76.950	69.834	28.830	1.00	77.23
ATOM	1572	CD	GLU	A	990	76.930	70.244	30.322	1.00	77.23
ATOM	1573	OE1	GLU	A	990	77.431	69.468	31.165	1.00	77.23
ATOM	1574	OE2	GLU	A	990	76.406	71.337	30.658	1.00	77.23
ATOM	1576	N	VAL	A	991	75.946	68.228	25.727	1.00	24.20
ATOM	1577	CA	VAL	A	991	75.831	68.569	24.274	1.00	24.20
ATOM	1578	C	VAL	A	991	75.272	69.989	24.073	1.00	24.20
ATOM	1579	O	VAL	A	991	75.089	70.682	25.017	1.00	24.20
ATOM	1580	CB	VAL	A	991	74.897	67.572	23.527	1.00	55.15
ATOM	1581	CG1	VAL	A	991	75.197	67.520	22.035	1.00	55.15
ATOM	1582	CG2	VAL	A	991	75.015	66.252	24.148	1.00	55.15
ATOM	1584	N	TYR	A	992	75.056	70.398	22.840	1.00	53.40
ATOM	1585	CA	TYR	A	992	74.514	71.693	22.545	1.00	53.40
ATOM	1586	C	TYR	A	992	73.954	71.659	21.140	1.00	53.40
ATOM	1587	O	TYR	A	992	74.678	71.455	20.177	1.00	53.40
ATOM	1588	CB	TYR	A	992	75.594	72.774	22.658	1.00	83.17
ATOM	1589	CG	TYR	A	992	75.167	74.067	22.018	1.00	83.17
ATOM	1590	CD1	TYR	A	992	74.337	74.950	22.688	1.00	83.17
ATOM	1591	CD2	TYR	A	992	75.452	74.316	20.694	1.00	83.17
ATOM	1592	CE1	TYR	A	992	73.796	76.025	22.047	1.00	83.17
ATOM	1593	CE2	TYR	A	992	74.919	75.380	20.053	1.00	83.17
ATOM	1594	CZ	TYR	A	992	74.090	76.230	20.726	1.00	83.17
ATOM	1595	OH	TYR	A	992	73.569	77.297	20.053	1.00	83.17
ATOM	1598	N	VAL	A	993	72.645	71.821	21.015	1.00	100.00
ATOM	1599	CA	VAL	A	993	72.047	71.808	19.695	1.00	100.00
ATOM	1600	C	VAL	A	993	70.897	72.813	19.594	1.00	100.00
ATOM	1601	O	VAL	A	993	69.736	72.514	19.912	1.00	100.00
ATOM	1602	CB	VAL	A	993	71.604	70.371	19.304	1.00	80.14
ATOM	1603	CG1	VAL	A	993	71.422	69.529	20.538	1.00	80.14
ATOM	1604	CG2	VAL	A	993	70.338	70.409	18.450	1.00	80.14
ATOM	1606	N	LYS	A	994	71.260	74.022	19.155	1.00	83.98
ATOM	1607	CA	LYS	A	994	70.329	75.125	18.980	1.00	83.98
ATOM	1608	C	LYS	A	994	69.729	74.959	17.615	1.00	83.98
ATOM	1609	O	LYS	A	994	70.421	74.538	16.688	1.00	83.98
ATOM	1610	CB	LYS	A	994	71.076	76.455	19.070	1.00	100.00
ATOM	1611	CG	LYS	A	994	70.350	77.670	18.498	1.00	100.00
ATOM	1612	CD	LYS	A	994	71.347	78.789	18.226	1.00	100.00

FIG. 6W

ATOM	1613	CE	LYS	A	994	70.694	80.150	18.153	1.00	100.00
ATOM	1614	NZ	LYS	A	994	71.425	81.159	18.962	1.00	100.00
ATOM	1619	N	LYS	A	995	68.446	75.287	17.488	1.00	66.77
ATOM	1620	CA	LYS	A	995	67.741	75.142	16.210	1.00	66.77
ATOM	1621	C	LYS	A	995	68.023	73.749	15.591	1.00	66.77
ATOM	1622	O	LYS	A	995	67.910	73.583	14.358	1.00	66.77
ATOM	1623	CB	LYS	A	995	68.167	76.265	15.244	1.00	100.00
ATOM	1624	OXT	LYS	A	995	68.354	72.815	16.355	1.00	100.00
ATOM	1626	N	PRO	A	1001	61.032	69.682	22.189	1.00	23.57
ATOM	1627	CA	PRO	A	1001	59.754	69.092	22.679	1.00	23.57
ATOM	1628	C	PRO	A	1001	59.681	69.765	24.004	1.00	23.57
ATOM	1629	O	PRO	A	1001	59.857	69.162	25.026	1.00	23.57
ATOM	1630	CB	PRO	A	1001	59.964	67.607	22.863	1.00	82.24
ATOM	1631	CG	PRO	A	1001	61.529	67.446	22.804	1.00	82.24
ATOM	1632	CD	PRO	A	1001	62.179	68.812	22.494	1.00	82.24
ATOM	1635	N	VAL	A	1002	59.429	71.067	23.965	1.00	14.96
ATOM	1636	CA	VAL	A	1002	59.401	71.905	25.163	1.00	14.96
ATOM	1637	C	VAL	A	1002	58.731	71.247	26.277	1.00	14.96
ATOM	1638	O	VAL	A	1002	58.930	71.607	27.409	1.00	14.96
ATOM	1639	CB	VAL	A	1002	58.755	73.268	24.833	1.00	66.63
ATOM	1640	CG1	VAL	A	1002	57.691	73.065	23.764	1.00	66.63
ATOM	1641	CG2	VAL	A	1002	58.212	73.946	26.088	1.00	66.63
ATOM	1643	N	ARG	A	1003	57.913	70.256	25.990	1.00	36.10
ATOM	1644	CA	ARG	A	1003	57.188	69.580	27.054	1.00	36.10
ATOM	1645	C	ARG	A	1003	57.957	68.409	27.649	1.00	36.10
ATOM	1646	O	ARG	A	1003	57.762	68.012	28.773	1.00	36.10
ATOM	1647	CB	ARG	A	1003	55.829	69.195	26.507	1.00	97.10
ATOM	1648	CG	ARG	A	1003	55.381	70.237	25.495	1.00	97.10
ATOM	1649	CD	ARG	A	1003	53.974	70.007	25.036	1.00	97.10
ATOM	1650	NE	ARG	A	1003	53.022	70.432	26.045	1.00	97.10
ATOM	1651	CZ	ARG	A	1003	51.949	71.153	25.782	1.00	97.10
ATOM	1652	NH1	ARG	A	1003	51.699	71.527	24.544	1.00	97.10
ATOM	1653	NH2	ARG	A	1003	51.136	71.493	26.759	1.00	97.10
ATOM	1660	N	TRP	A	1004	58.902	67.934	26.865	1.00	31.39
ATOM	1661	CA	TRP	A	1004	59.799	66.858	27.231	1.00	31.39
ATOM	1662	C	TRP	A	1004	61.031	67.342	27.941	1.00	31.39
ATOM	1663	O	TRP	A	1004	61.431	66.841	28.992	1.00	31.39
ATOM	1664	CB	TRP	A	1004	60.117	66.113	25.981	1.00	37.57
ATOM	1665	CG	TRP	A	1004	59.058	65.128	25.860	1.00	37.57
ATOM	1666	CD1	TRP	A	1004	59.055	63.870	26.415	1.00	37.57
ATOM	1667	CD2	TRP	A	1004	57.758	65.324	25.323	1.00	37.57
ATOM	1668	NE1	TRP	A	1004	57.832	63.290	26.253	1.00	37.57
ATOM	1669	CE2	TRP	A	1004	57.011	64.149	25.594	1.00	37.57
ATOM	1670	CE3	TRP	A	1004	57.142	66.370	24.648	1.00	37.57
ATOM	1671	CZ2	TRP	A	1004	55.683	63.991	25.214	1.00	37.57
ATOM	1672	CZ3	TRP	A	1004	55.789	66.223	24.252	1.00	37.57
ATOM	1673	CH2	TRP	A	1004	55.087	65.041	24.541	1.00	37.57
ATOM	1676	N	MET	A	1005	61.556	68.426	27.391	1.00	10.72
ATOM	1677	CA	MET	A	1005	62.723	69.067	27.879	1.00	10.72
ATOM	1678	C	MET	A	1005	62.709	69.405	29.340	1.00	10.72
ATOM	1679	O	MET	A	1005	61.690	69.822	29.947	1.00	10.72
ATOM	1680	CB	MET	A	1005	62.983	70.254	27.003	1.00	63.30
ATOM	1681	CG	MET	A	1005	63.299	69.783	25.632	1.00	63.30
ATOM	1682	SD	MET	A	1005	63.194	71.078	24.467	1.00	63.30
ATOM	1683	CE	MET	A	1005	64.494	72.111	25.002	1.00	63.30
ATOM	1685	N	ALA	A	1006	63.873	69.180	29.939	1.00	13.71
ATOM	1686	CA	ALA	A	1006	64.092	69.541	31.343	1.00	13.71

FIG. 6X

ATOM	1687	C	ALA	A1006	64.634	71.015	31.321	1.00	13.71
ATOM	1688	O	ALA	A1006	64.885	71.575	30.254	1.00	13.71
ATOM	1689	CB	ALA	A1006	65.114	68.618	31.976	1.00	44.23
ATOM	1691	N	ILE	A1007	64.762	71.597	32.515	1.00	21.54
ATOM	1692	CA	ILE	A1007	65.278	72.951	32.738	1.00	21.54
ATOM	1693	C	ILE	A1007	66.586	73.324	31.943	1.00	21.54
ATOM	1694	O	ILE	A1007	66.528	73.791	30.817	1.00	21.54
ATOM	1695	CB	ILE	A1007	65.482	73.137	34.300	1.00	20.90
ATOM	1696	CG1	ILE	A1007	66.672	72.188	34.830	1.00	20.90
ATOM	1697	CG2	ILE	A1007	64.088	72.800	35.034	1.00	20.90
ATOM	1698	CD1	ILE	A1007	67.395	72.474	36.237	1.00	20.90
ATOM	1700	N	GLU	A1008	67.752	73.082	32.510	1.00	10.72
ATOM	1701	CA	GLU	A1008	69.028	73.410	31.892	1.00	10.72
ATOM	1702	C	GLU	A1008	69.066	73.404	30.369	1.00	10.72
ATOM	1703	O	GLU	A1008	70.144	73.771	29.757	1.00	10.72
ATOM	1704	CB	GLU	A1008	70.098	72.429	32.417	1.00	39.30
ATOM	1705	CG	GLU	A1008	69.942	70.977	31.916	1.00	39.30
ATOM	1706	CD	GLU	A1008	69.159	70.091	32.896	1.00	39.30
ATOM	1707	OE1	GLU	A1008	68.082	70.549	33.382	1.00	39.30
ATOM	1708	OE2	GLU	A1008	69.634	68.944	33.178	1.00	39.30
ATOM	1710	N	SER	A1009	67.976	72.880	29.764	1.00	31.45
ATOM	1711	CA	SER	A1009	67.798	72.791	28.314	1.00	31.45
ATOM	1712	C	SER	A1009	66.826	73.844	27.779	1.00	31.45
ATOM	1713	O	SER	A1009	67.007	74.396	26.685	1.00	31.45
ATOM	1714	CB	SER	A1009	67.286	71.410	27.930	1.00	100.00
ATOM	1715	OG	SER	A1009	68.088	70.402	28.500	1.00	100.00
ATOM	1718	N	LEU	A1010	65.745	74.095	28.485	1.00	75.06
ATOM	1719	CA	LEU	A1010	64.852	75.103	27.977	1.00	75.06
ATOM	1720	C	LEU	A1010	65.758	76.342	27.926	1.00	75.06
ATOM	1721	O	LEU	A1010	65.737	77.146	26.989	1.00	75.06
ATOM	1722	CB	LEU	A1010	63.675	75.238	28.938	1.00	62.28
ATOM	1723	CG	LEU	A1010	62.685	74.078	28.725	1.00	62.28
ATOM	1724	CD1	LEU	A1010	61.421	74.394	29.511	1.00	62.28
ATOM	1725	CD2	LEU	A1010	62.379	73.854	27.229	1.00	62.28
ATOM	1727	N	ASN	A1011	66.597	76.401	28.951	1.00	36.75
ATOM	1728	CA	ASN	A1011	67.611	77.389	29.207	1.00	36.75
ATOM	1729	C	ASN	A1011	68.761	77.280	28.189	1.00	36.75
ATOM	1730	O	ASN	A1011	68.696	77.728	27.006	1.00	36.75
ATOM	1731	CB	ASN	A1011	68.174	77.122	30.588	1.00	53.79
ATOM	1732	CG	ASN	A1011	67.148	77.215	31.633	1.00	53.79
ATOM	1733	OD1	ASN	A1011	66.008	77.430	31.335	1.00	53.79
ATOM	1734	ND2	ASN	A1011	67.541	77.071	32.879	1.00	53.79
ATOM	1738	N	TYR	A1012	69.810	76.638	28.685	1.00	25.53
ATOM	1739	CA	TYR	A1012	71.016	76.422	27.940	1.00	25.53
ATOM	1740	C	TYR	A1012	70.747	75.476	26.776	1.00	25.53
ATOM	1741	O	TYR	A1012	71.392	75.570	25.756	1.00	25.53
ATOM	1742	CB	TYR	A1012	72.118	75.898	28.872	1.00	38.16
ATOM	1743	CG	TYR	A1012	71.934	76.312	30.315	1.00	38.16
ATOM	1744	CD1	TYR	A1012	72.332	75.491	31.341	1.00	38.16
ATOM	1745	CD2	TYR	A1012	71.301	77.512	30.645	1.00	38.16
ATOM	1746	CE1	TYR	A1012	72.105	75.841	32.642	1.00	38.16
ATOM	1747	CE2	TYR	A1012	71.072	77.863	31.943	1.00	38.16
ATOM	1748	CZ	TYR	A1012	71.473	77.028	32.927	1.00	38.16
ATOM	1749	OH	TYR	A1012	71.240	77.363	34.217	1.00	38.16
ATOM	1752	N	SER	A1013	69.812	74.566	26.863	1.00	71.42
ATOM	1753	CA	SER	A1013	69.638	73.752	25.672	1.00	71.42
ATOM	1754	C	SER	A1013	70.875	72.864	25.398	1.00	71.42

FIG. 6Y

ATOM	1755	O	SER	A1013	71.360	72.693	24.272	1.00	71.42
ATOM	1756	CB	SER	A1013	69.331	74.696	24.502	1.00	25.42
ATOM	1757	OG	SER	A1013	70.477	75.126	23.819	1.00	25.42
ATOM	1760	N	VAL	A1014	71.383	72.310	26.482	1.00	66.71
ATOM	1761	CA	VAL	A1014	72.507	71.433	26.395	1.00	66.71
ATOM	1762	C	VAL	A1014	71.902	70.215	26.967	1.00	66.71
ATOM	1763	O	VAL	A1014	71.255	70.283	27.994	1.00	66.71
ATOM	1764	CB	VAL	A1014	73.745	71.888	27.263	1.00	53.96
ATOM	1765	CG1	VAL	A1014	74.220	73.271	26.795	1.00	53.96
ATOM	1766	CG2	VAL	A1014	73.427	71.814	28.765	1.00	53.96
ATOM	1768	N	TYR	A1015	72.067	69.104	26.273	1.00	65.68
ATOM	1769	CA	TYR	A1015	71.511	67.861	26.751	1.00	65.68
ATOM	1770	C	TYR	A1015	72.584	66.891	27.248	1.00	65.68
ATOM	1771	O	TYR	A1015	73.635	66.702	26.646	1.00	65.68
ATOM	1772	CB	TYR	A1015	70.656	67.214	25.663	1.00	100.00
ATOM	1773	CG	TYR	A1015	69.758	68.179	24.939	1.00	100.00
ATOM	1774	CD1	TYR	A1015	70.148	68.741	23.734	1.00	100.00
ATOM	1775	CD2	TYR	A1015	68.509	68.505	25.434	1.00	100.00
ATOM	1776	CE1	TYR	A1015	69.315	69.596	23.037	1.00	100.00
ATOM	1777	CE2	TYR	A1015	67.664	69.364	24.740	1.00	100.00
ATOM	1778	CZ	TYR	A1015	68.078	69.901	23.546	1.00	100.00
ATOM	1779	OH	TYR	A1015	67.272	70.751	22.848	1.00	100.00
ATOM	1782	N	THR	A1016	72.263	66.269	28.363	1.00	55.88
ATOM	1783	CA	THR	A1016	73.124	65.322	29.008	1.00	55.88
ATOM	1784	C	THR	A1016	72.360	64.056	29.380	1.00	55.88
ATOM	1785	O	THR	A1016	71.164	63.996	29.243	1.00	55.88
ATOM	1786	CB	THR	A1016	73.653	65.988	30.209	1.00	30.90
ATOM	1787	OG1	THR	A1016	72.699	65.891	31.280	1.00	30.90
ATOM	1788	CG2	THR	A1016	73.881	67.440	29.876	1.00	30.90
ATOM	1791	N	THR	A1017	73.054	63.037	29.840	1.00	99.25
ATOM	1792	CA	THR	A1017	72.361	61.822	30.213	1.00	99.25
ATOM	1793	C	THR	A1017	71.878	62.074	31.618	1.00	99.25
ATOM	1794	O	THR	A1017	72.112	61.294	32.534	1.00	99.25
ATOM	1795	CB	THR	A1017	73.312	60.593	30.094	1.00	32.66
ATOM	1796	OG1	THR	A1017	72.893	59.789	28.972	1.00	32.66
ATOM	1797	CG2	THR	A1017	73.353	59.770	31.323	1.00	32.66
ATOM	1800	N	ASN	A1018	71.185	63.198	31.786	1.00	18.01
ATOM	1801	CA	ASN	A1018	70.687	63.569	33.141	1.00	18.01
ATOM	1802	C	ASN	A1018	69.349	64.119	32.874	1.00	18.01
ATOM	1803	O	ASN	A1018	68.447	64.021	33.724	1.00	18.01
ATOM	1804	CB	ASN	A1018	71.527	64.623	33.742	1.00	34.98
ATOM	1805	GG	ASN	A1018	71.808	64.337	35.101	1.00	34.98
ATOM	1806	OD1	ASN	A1018	71.282	64.966	35.982	1.00	34.98
ATOM	1807	ND2	ASN	A1018	72.659	63.353	35.331	1.00	34.98
ATOM	1811	N	SER	A1019	69.294	64.679	31.656	1.00	37.97
ATOM	1812	CA	SER	A1019	68.205	65.335	30.991	1.00	37.97
ATOM	1813	C	SER	A1019	67.811	64.369	29.862	1.00	37.97
ATOM	1814	O	SER	A1019	67.493	64.733	28.729	1.00	37.97
ATOM	1815	CB	SER	A1019	68.737	66.641	30.420	1.00	17.17
ATOM	1816	OG	SER	A1019	69.329	66.474	29.138	1.00	17.17
ATOM	1819	N	ASP	A1020	67.985	63.097	30.155	1.00	31.25
ATOM	1820	CA	ASP	A1020	67.582	62.062	29.225	1.00	31.25
ATOM	1821	C	ASP	A1020	66.669	61.475	30.328	1.00	31.25
ATOM	1822	O	ASP	A1020	65.473	61.257	30.127	1.00	31.25
ATOM	1823	CB	ASP	A1020	68.777	61.166	28.790	1.00	31.83
ATOM	1824	CG	ASP	A1020	69.074	61.295	27.302	1.00	31.83
ATOM	1825	OD1	ASP	A1020	68.289	61.870	26.618	1.00	31.83

FIG. 6Z

ATOM	1826	OD2	ASP	A1020	70.043	60.869	26.709	1.00	31.83
ATOM	1828	N	VAL	A1021	67.214	61.357	31.535	1.00	57.04
ATOM	1829	CA	VAL	A1021	66.440	60.813	32.614	1.00	57.04
ATOM	1830	C	VAL	A1021	65.131	61.522	32.628	1.00	57.04
ATOM	1831	O	VAL	A1021	64.091	60.915	32.317	1.00	57.04
ATOM	1832	CB	VAL	A1021	67.130	60.987	33.916	1.00	94.63
ATOM	1833	CG1	VAL	A1021	66.156	60.813	35.032	1.00	94.63
ATOM	1834	CG2	VAL	A1021	68.236	59.965	34.012	1.00	94.63
ATOM	1836	N	TRP	A1022	65.189	62.814	32.960	1.00	51.41
ATOM	1837	CA	TRP	A1022	64.023	63.696	33.032	1.00	51.41
ATOM	1838	C	TRP	A1022	63.002	63.457	31.908	1.00	51.41
ATOM	1839	O	TRP	A1022	61.815	63.252	32.147	1.00	51.41
ATOM	1840	CB	TRP	A1022	64.519	65.133	33.005	1.00	32.10
ATOM	1841	CG	TRP	A1022	63.422	66.227	32.925	1.00	32.10
ATOM	1842	CD1	TRP	A1022	62.602	66.469	31.868	1.00	32.10
ATOM	1843	CD2	TRP	A1022	63.068	67.160	33.938	1.00	32.10
ATOM	1844	NE1	TRP	A1022	61.779	67.469	32.157	1.00	32.10
ATOM	1845	CE2	TRP	A1022	62.032	67.931	33.428	1.00	32.10
ATOM	1846	CE3	TRP	A1022	63.526	67.420	35.221	1.00	32.10
ATOM	1847	CZ2	TRP	A1022	61.408	69.004	34.187	1.00	32.10
ATOM	1848	CZ3	TRP	A1022	62.921	68.481	35.978	1.00	32.10
ATOM	1849	CH2	TRP	A1022	61.879	69.255	35.453	1.00	32.10
ATOM	1852	N	SER	A1023	63.472	63.525	30.671	1.00	66.03
ATOM	1853	CA	SER	A1023	62.598	63.263	29.546	1.00	66.03
ATOM	1854	C	SER	A1023	61.921	61.955	29.911	1.00	66.03
ATOM	1855	O	SER	A1023	60.717	61.903	30.036	1.00	66.03
ATOM	1856	CB	SER	A1023	63.414	63.109	28.274	1.00	96.89
ATOM	1857	OG	SER	A1023	63.734	64.377	27.752	1.00	96.89
ATOM	1860	N	TYR	A1024	62.719	60.909	30.106	1.00	11.41
ATOM	1861	CA	TYR	A1024	62.238	59.645	30.472	1.00	11.41
ATOM	1862	C	TYR	A1024	60.940	59.597	31.308	1.00	11.41
ATOM	1863	O	TYR	A1024	60.018	58.807	30.992	1.00	11.41
ATOM	1864	CB	TYR	A1024	63.320	58.871	31.188	1.00	14.38
ATOM	1865	CG	TYR	A1024	62.850	57.491	31.472	1.00	14.38
ATOM	1866	CD1	TYR	A1024	62.821	56.581	30.474	1.00	14.38
ATOM	1867	CD2	TYR	A1024	62.314	57.167	32.733	1.00	14.38
ATOM	1868	CE1	TYR	A1024	62.276	55.380	30.688	1.00	14.38
ATOM	1869	CE2	TYR	A1024	61.765	55.987	32.993	1.00	14.38
ATOM	1870	CZ	TYR	A1024	61.734	55.069	31.972	1.00	14.38
ATOM	1871	OH	TYR	A1024	61.197	53.831	32.179	1.00	14.38
ATOM	1874	N	GLY	A1025	60.894	60.341	32.397	1.00	29.83
ATOM	1875	CA	GLY	A1025	59.678	60.385	33.207	1.00	29.83
ATOM	1876	C	GLY	A1025	58.509	61.033	32.430	1.00	29.83
ATOM	1877	O	GLY	A1025	57.356	60.716	32.652	1.00	29.83
ATOM	1879	N	VAL	A1026	58.762	61.985	31.554	1.00	67.56
ATOM	1880	CA	VAL	A1026	57.615	62.466	30.859	1.00	67.56
ATOM	1881	C	VAL	A1026	57.199	61.121	30.271	1.00	67.56
ATOM	1882	O	VAL	A1026	56.204	60.589	30.705	1.00	67.56
ATOM	1883	CB	VAL	A1026	57.975	63.548	29.836	1.00	59.88
ATOM	1884	CG1	VAL	A1026	56.872	64.579	29.759	1.00	59.88
ATOM	1885	CG2	VAL	A1026	59.232	64.199	30.249	1.00	59.88
ATOM	1887	N	LEU	A1027	57.982	60.546	29.354	1.00	31.95
ATOM	1888	CA	LEU	A1027	57.703	59.178	28.787	1.00	31.95
ATOM	1889	C	LEU	A1027	57.056	58.236	29.865	1.00	31.95
ATOM	1890	O	LEU	A1027	55.988	57.621	29.691	1.00	31.95
ATOM	1891	CB	LEU	A1027	59.000	58.502	28.304	1.00	37.14
ATOM	1892	CG	LEU	A1027	58.894	57.447	27.219	1.00	37.14

FIG. 6AA

ATOM	1893	CD1	LEU	A1027	57.496	57.117	27.007	1.00	37.14
ATOM	1894	CD2	LEU	A1027	59.417	57.890	25.930	1.00	37.14
ATOM	1896	N	LEU	A1028	57.746	58.125	30.978	1.00	8.77
ATOM	1897	CA	LEU	A1028	57.188	57.363	32.009	1.00	8.77
ATOM	1898	C	LEU	A1028	55.743	57.749	32.088	1.00	8.77
ATOM	1899	O	LEU	A1028	54.947	56.870	31.744	1.00	8.77
ATOM	1900	CB	LEU	A1028	57.875	57.508	33.363	1.00	48.45
ATOM	1901	CG	LEU	A1028	57.252	56.440	34.294	1.00	48.45
ATOM	1902	CD1	LEU	A1028	56.823	55.185	33.534	1.00	48.45
ATOM	1903	CD2	LEU	A1028	58.220	56.043	35.333	1.00	48.45
ATOM	1905	N	TRP	A1029	55.442	59.029	32.483	1.00	30.07
ATOM	1906	CA	TRP	A1029	54.084	59.703	32.660	1.00	30.07
ATOM	1907	C	TRP	A1029	53.253	59.613	31.429	1.00	30.07
ATOM	1908	O	TRP	A1029	52.118	59.261	31.397	1.00	30.07
ATOM	1909	CB	TRP	A1029	54.227	61.222	32.983	1.00	2.92
ATOM	1910	CG	TRP	A1029	52.932	62.000	33.312	1.00	2.92
ATOM	1911	CD1	TRP	A1029	52.349	62.276	34.582	1.00	2.92
ATOM	1912	CD2	TRP	A1029	51.964	62.434	32.334	1.00	2.92
ATOM	1913	NE1	TRP	A1029	51.050	62.846	34.369	1.00	2.92
ATOM	1914	CE2	TRP	A1029	50.827	62.919	33.011	1.00	2.92
ATOM	1915	CE3	TRP	A1029	51.955	62.444	30.937	1.00	2.92
ATOM	1916	CZ2	TRP	A1029	49.767	63.362	32.342	1.00	2.92
ATOM	1917	CZ3	TRP	A1029	50.836	62.910	30.283	1.00	2.92
ATOM	1918	CH2	TRP	A1029	49.791	63.345	30.971	1.00	2.92
ATOM	1921	N	GLU	A1030	53.881	60.008	30.382	1.00	26.20
ATOM	1922	CA	GLU	A1030	53.292	59.957	29.076	1.00	26.20
ATOM	1923	C	GLU	A1030	52.824	58.589	28.725	1.00	26.20
ATOM	1924	O	GLU	A1030	52.344	58.417	27.638	1.00	26.20
ATOM	1925	CB	GLU	A1030	54.358	60.378	28.077	1.00	24.00
ATOM	1926	CG	GLU	A1030	53.879	60.996	26.869	1.00	24.00
ATOM	1927	CD	GLU	A1030	54.860	60.718	25.857	1.00	24.00
ATOM	1928	OE1	GLU	A1030	55.885	60.279	26.378	1.00	24.00
ATOM	1929	OE2	GLU	A1030	54.661	60.907	24.633	1.00	24.00
ATOM	1931	N	ILE	A1031	52.969	57.631	29.631	1.00	14.69
ATOM	1932	CA	ILE	A1031	52.633	56.216	29.376	1.00	14.69
ATOM	1933	C	ILE	A1031	51.704	55.738	30.426	1.00	14.69
ATOM	1934	O	ILE	A1031	51.033	54.761	30.203	1.00	14.69
ATOM	1935	CB	ILE	A1031	53.923	55.272	29.416	1.00	33.44
ATOM	1936	CG1	ILE	A1031	54.294	54.757	28.021	1.00	33.44
ATOM	1937	CG2	ILE	A1031	53.671	53.993	30.253	1.00	33.44
ATOM	1938	CD1	ILE	A1031	55.762	54.225	27.948	1.00	33.44
ATOM	1940	N	VAL	A1032	51.726	56.285	31.621	1.00	14.19
ATOM	1941	CA	VAL	A1032	50.676	55.868	32.559	1.00	14.19
ATOM	1942	C	VAL	A1032	49.327	56.496	32.011	1.00	14.19
ATOM	1943	O	VAL	A1032	48.282	55.823	31.882	1.00	14.19
ATOM	1944	CB	VAL	A1032	50.924	56.349	33.944	1.00	41.51
ATOM	1945	CG1	VAL	A1032	49.666	56.640	34.596	1.00	41.51
ATOM	1946	CG2	VAL	A1032	51.581	55.290	34.704	1.00	41.51
ATOM	1948	N	SER	A1033	49.395	57.755	31.625	1.00	31.81
ATOM	1949	CA	SER	A1033	48.320	58.505	31.065	1.00	31.81
ATOM	1950	C	SER	A1033	47.658	57.730	29.910	1.00	31.81
ATOM	1951	O	SER	A1033	46.551	58.079	29.445	1.00	31.81
ATOM	1952	CB	SER	A1033	48.895	59.828	30.546	1.00	68.54
ATOM	1953	OG	SER	A1033	49.757	59.623	29.445	1.00	68.54
ATOM	1956	N	LEU	A1034	48.316	56.686	29.442	1.00	2.00
ATOM	1957	CA	LEU	A1034	47.777	55.984	28.298	1.00	2.00
ATOM	1958	C	LEU	A1034	47.645	56.833	26.999	1.00	2.00

FIG. 6BB

ATOM	1959	O	LEU	A1034	46.584	56.955	26.409	1.00	2.00
ATOM	1960	CB	LEU	A1034	46.422	55.343	28.654	1.00	31.43
ATOM	1961	CG	LEU	A1034	46.478	53.883	29.207	1.00	31.43
ATOM	1962	CD1	LEU	A1034	45.072	53.333	29.484	1.00	31.43
ATOM	1963	CD2	LEU	A1034	47.244	52.988	28.207	1.00	31.43
ATOM	1965	N	GLY	A1035	48.706	57.372	26.438	1.00	4.53
ATOM	1966	CA	GLY	A1035	48.437	58.149	25.224	1.00	4.53
ATOM	1967	C	GLY	A1035	48.241	59.685	25.565	1.00	4.53
ATOM	1968	O	GLY	A1035	47.964	60.498	24.649	1.00	4.53
ATOM	1970	N	GLY	A1036	48.509	60.071	26.820	1.00	18.31
ATOM	1971	CA	GLY	A1036	48.281	61.470	27.160	1.00	18.31
ATOM	1972	C	GLY	A1036	49.211	62.717	27.185	1.00	18.31
ATOM	1973	O	GLY	A1036	49.988	62.881	28.181	1.00	18.31
ATOM	1975	N	THR	A1037	49.027	63.591	26.164	1.00	48.85
ATOM	1976	CA	THR	A1037	49.733	64.890	25.939	1.00	48.85
ATOM	1977	C	THR	A1037	50.225	65.522	27.265	1.00	48.85
ATOM	1978	O	THR	A1037	49.431	65.933	28.077	1.00	48.85
ATOM	1979	CB	THR	A1037	48.780	65.886	25.216	1.00	25.15
ATOM	1980	OG1	THR	A1037	48.988	65.904	23.772	1.00	25.15
ATOM	1981	CG2	THR	A1037	48.993	67.215	25.789	1.00	25.15
ATOM	1984	N	PRO	A1038	51.538	65.697	27.456	1.00	42.23
ATOM	1985	CA	PRO	A1038	51.796	66.239	28.775	1.00	42.23
ATOM	1986	C	PRO	A1038	51.496	67.691	28.996	1.00	42.23
ATOM	1987	O	PRO	A1038	51.359	68.450	28.057	1.00	42.23
ATOM	1988	CB	PRO	A1038	53.271	65.779	29.048	1.00	10.66
ATOM	1989	CG	PRO	A1038	53.679	65.007	27.861	1.00	10.66
ATOM	1990	CD	PRO	A1038	52.809	65.456	26.765	1.00	10.66
ATOM	1991	N	TYR	A1039	51.381	68.090	30.253	1.00	39.67
ATOM	1992	CA	TYR	A1039	51.037	69.509	30.576	1.00	39.67
ATOM	1993	C	TYR	A1039	49.924	69.987	29.682	1.00	39.67
ATOM	1994	O	TYR	A1039	50.172	70.931	28.955	1.00	39.67
ATOM	1995	CB	TYR	A1039	52.256	70.457	30.375	1.00	15.36
ATOM	1996	CG	TYR	A1039	53.503	69.958	31.103	1.00	15.36
ATOM	1997	CD1	TYR	A1039	54.685	69.536	30.407	1.00	15.36
ATOM	1998	CD2	TYR	A1039	53.518	69.952	32.481	1.00	15.36
ATOM	1999	CE1	TYR	A1039	55.790	69.157	31.105	1.00	15.36
ATOM	2000	CE2	TYR	A1039	54.636	69.571	33.153	1.00	15.36
ATOM	2001	CZ	TYR	A1039	55.737	69.191	32.449	1.00	15.36
ATOM	2002	OH	TYR	A1039	56.737	68.889	33.251	1.00	15.36
ATOM	2005	N	CYS	A1040	48.756	69.319	29.692	1.00	100.00
ATOM	2006	CA	CYS	A1040	47.597	69.681	28.845	1.00	100.00
ATOM	2007	C	CYS	A1040	47.013	70.930	29.435	1.00	100.00
ATOM	2008	O	CYS	A1040	46.711	70.987	30.625	1.00	100.00
ATOM	2009	CB	CYS	A1040	46.507	68.566	28.832	1.00	63.76
ATOM	2010	SG	CYS	A1040	45.039	68.722	27.619	1.00	63.76
ATOM	2012	N	GLY	A1041	46.836	71.938	28.605	1.00	75.53
ATOM	2013	CA	GLY	A1041	46.305	73.175	29.127	1.00	75.53
ATOM	2014	C	GLY	A1041	47.419	74.160	29.448	1.00	75.53
ATOM	2015	O	GLY	A1041	47.217	75.358	29.342	1.00	75.53
ATOM	2017	N	MET	A1042	48.581	73.668	29.868	1.00	27.54
ATOM	2018	CA	MET	A1042	49.666	74.553	30.126	1.00	27.54
ATOM	2019	C	MET	A1042	50.119	75.065	28.731	1.00	27.54
ATOM	2020	O	MET	A1042	50.034	74.344	27.742	1.00	27.54
ATOM	2021	CB	MET	A1042	50.771	73.851	30.909	1.00	47.82
ATOM	2022	CG	MET	A1042	51.032	74.460	32.298	1.00	47.82
ATOM	2023	SD	MET	A1042	52.810	74.502	32.805	1.00	47.82
ATOM	2024	CE	MET	A1042	52.729	74.790	34.564	1.00	47.82

FIG. 6CC

ATOM	2026	N	THR	A1043	50.481	76.351	28.681	1.00	59.25
ATOM	2027	CA	THR	A1043	50.918	77.067	27.468	1.00	59.25
ATOM	2028	C	THR	A1043	52.434	76.937	27.397	1.00	59.25
ATOM	2029	O	THR	A1043	53.084	76.835	28.437	1.00	59.25
ATOM	2030	CB	THR	A1043	50.586	78.617	27.528	1.00	62.50
ATOM	2031	OG1	THR	A1043	51.070	79.181	28.773	1.00	62.50
ATOM	2032	CG2	THR	A1043	49.076	78.877	27.351	1.00	62.50
ATOM	2035	N	CYS	A1044	52.997	76.968	26.194	1.00	100.00
ATOM	2036	CA	CYS	A1044	54.435	76.799	26.060	1.00	100.00
ATOM	2037	C	CYS	A1044	55.282	77.679	26.975	1.00	100.00
ATOM	2038	O	CYS	A1044	56.478	77.467	27.100	1.00	100.00
ATOM	2039	CB	CYS	A1044	54.857	76.963	24.601	1.00	77.67
ATOM	2040	SG	CYS	A1044	54.890	75.383	23.687	1.00	77.67
ATOM	2042	N	ALA	A1045	54.673	78.663	27.623	1.00	100.00
ATOM	2043	CA	ALA	A1045	55.425	79.501	28.548	1.00	100.00
ATOM	2044	C	ALA	A1045	54.810	79.446	29.910	1.00	100.00
ATOM	2045	O	ALA	A1045	55.455	79.833	30.878	1.00	100.00
ATOM	2046	CB	ALA	A1045	55.461	80.899	28.107	1.00	35.04
ATOM	2048	N	GLU	A1046	53.550	79.023	30.018	1.00	27.64
ATOM	2049	CA	GLU	A1046	53.057	78.932	31.346	1.00	27.64
ATOM	2050	C	GLU	A1046	54.177	78.018	31.917	1.00	27.64
ATOM	2051	O	GLU	A1046	54.507	78.117	33.092	1.00	27.64
ATOM	2052	CB	GLU	A1046	51.665	78.264	31.365	1.00	79.70
ATOM	2053	CG	GLU	A1046	50.465	79.239	31.521	1.00	79.70
ATOM	2054	CD	GLU	A1046	49.180	78.818	30.745	1.00	79.70
ATOM	2055	OE1	GLU	A1046	48.058	79.216	31.128	1.00	79.70
ATOM	2056	OE2	GLU	A1046	49.264	78.096	29.748	1.00	79.70
ATOM	2058	N	LEU	A1047	54.800	77.199	31.050	1.00	83.80
ATOM	2059	CA	LEU	A1047	55.871	76.230	31.413	1.00	83.80
ATOM	2060	C	LEU	A1047	57.286	76.737	31.646	1.00	83.80
ATOM	2061	O	LEU	A1047	57.838	76.529	32.712	1.00	83.80
ATOM	2062	CB	LEU	A1047	55.968	75.119	30.368	1.00	39.62
ATOM	2063	CG	LEU	A1047	55.167	73.857	30.626	1.00	39.62
ATOM	2064	CD1	LEU	A1047	55.186	73.119	29.339	1.00	39.62
ATOM	2065	CD2	LEU	A1047	55.697	73.034	31.803	1.00	39.62
ATOM	2067	N	TYR	A1048	57.904	77.315	30.615	1.00	32.07
ATOM	2068	CA	TYR	A1048	59.235	77.894	30.746	1.00	32.07
ATOM	2069	C	TYR	A1048	59.043	78.647	32.109	1.00	32.07
ATOM	2070	O	TYR	A1048	59.704	78.383	33.115	1.00	32.07
ATOM	2071	CB	TYR	A1048	59.498	78.877	29.566	1.00	14.15
ATOM	2072	CG	TYR	A1048	60.160	78.333	28.256	1.00	14.15
ATOM	2073	CD1	TYR	A1048	59.401	77.982	27.165	1.00	14.15
ATOM	2074	CD2	TYR	A1048	61.563	78.249	28.095	1.00	14.15
ATOM	2075	CE1	TYR	A1048	59.969	77.565	25.934	1.00	14.15
ATOM	2076	CE2	TYR	A1048	62.137	77.841	26.871	1.00	14.15
ATOM	2077	CZ	TYR	A1048	61.359	77.502	25.784	1.00	14.15
ATOM	2078	OH	TYR	A1048	61.927	77.135	24.513	1.00	14.15
ATOM	2081	N	GLU	A1049	58.055	79.533	32.169	1.00	36.64
ATOM	2082	CA	GLU	A1049	57.811	80.267	33.390	1.00	36.64
ATOM	2083	C	GLU	A1049	57.770	79.384	34.578	1.00	36.64
ATOM	2084	O	GLU	A1049	58.757	79.290	35.320	1.00	36.64
ATOM	2085	CB	GLU	A1049	56.500	81.002	33.368	1.00	35.78
ATOM	2086	CG	GLU	A1049	56.151	81.544	34.760	1.00	35.78
ATOM	2087	CD	GLU	A1049	54.683	81.875	34.899	1.00	35.78
ATOM	2088	OE1	GLU	A1049	53.989	82.043	33.858	1.00	35.78
ATOM	2089	OE2	GLU	A1049	54.252	81.947	36.060	1.00	35.78
ATOM	2091	N	LYS	A1050	56.601	78.737	34.708	1.00	93.85

FIG. 6DD

ATOM	2092	CA	LYS	A1050	56.197	77.839	35.793	1.00	93.85
ATOM	2093	C	LYS	A1050	57.046	76.622	36.085	1.00	93.85
ATOM	2094	O	LYS	A1050	57.178	76.212	37.231	1.00	93.85
ATOM	2095	CB	LYS	A1050	54.752	77.418	35.584	1.00	86.89
ATOM	2097	N	LEU	A1051	57.599	76.008	35.063	1.00	40.78
ATOM	2098	CA	LEU	A1051	58.458	74.868	35.336	1.00	40.78
ATOM	2099	C	LEU	A1051	59.412	75.166	36.508	1.00	40.78
ATOM	2100	O	LEU	A1051	59.321	74.483	37.539	1.00	40.78
ATOM	2101	CB	LEU	A1051	59.201	74.391	34.072	1.00	66.80
ATOM	2102	CG	LEU	A1051	58.984	72.898	33.726	1.00	66.80
ATOM	2103	CD1	LEU	A1051	57.754	72.376	34.370	1.00	66.80
ATOM	2104	CD2	LEU	A1051	58.875	72.719	32.253	1.00	66.80
ATOM	2106	N	PRO	A1052	60.356	76.129	36.369	1.00	42.79
ATOM	2107	CA	PRO	A1052	61.299	76.504	37.431	1.00	42.79
ATOM	2108	C	PRO	A1052	60.655	76.803	38.741	1.00	42.79
ATOM	2109	O	PRO	A1052	61.311	76.783	39.783	1.00	42.79
ATOM	2110	CB	PRO	A1052	61.928	77.731	36.906	1.00	29.07
ATOM	2111	CG	PRO	A1052	61.952	77.549	35.473	1.00	29.07
ATOM	2112	CD	PRO	A1052	60.713	76.805	35.110	1.00	29.07
ATOM	2113	N	GLN	A1053	59.365	77.114	38.699	1.00	68.39
ATOM	2114	CA	GLN	A1053	58.662	77.426	39.921	1.00	68.39
ATOM	2115	C	GLN	A1053	58.823	76.206	40.781	1.00	68.39
ATOM	2116	O	GLN	A1053	58.934	76.303	41.999	1.00	68.39
ATOM	2117	CB	GLN	A1053	57.200	77.701	39.646	1.00	100.00
ATOM	2119	N	GLY	A1054	58.852	75.049	40.125	1.00	93.49
ATOM	2120	CA	GLY	A1054	59.012	73.776	40.808	1.00	93.49
ATOM	2121	C	GLY	A1054	57.849	72.863	40.494	1.00	93.49
ATOM	2122	O	GLY	A1054	57.727	71.794	41.065	1.00	93.49
ATOM	2124	N	TYR	A1055	57.000	73.311	39.577	1.00	23.98
ATOM	2125	CA	TYR	A1055	55.804	72.609	39.141	1.00	23.98
ATOM	2126	C	TYR	A1055	56.207	71.481	38.197	1.00	23.98
ATOM	2127	O	TYR	A1055	57.062	71.702	37.321	1.00	23.98
ATOM	2128	CB	TYR	A1055	54.869	73.579	38.415	1.00	76.79
ATOM	2129	CG	TYR	A1055	53.703	72.894	37.769	1.00	76.79
ATOM	2130	CD1	TYR	A1055	52.547	72.645	38.480	1.00	76.79
ATOM	2131	CD2	TYR	A1055	53.803	72.391	36.479	1.00	76.79
ATOM	2132	CE1	TYR	A1055	51.516	71.891	37.927	1.00	76.79
ATOM	2133	CE2	TYR	A1055	52.788	71.639	35.913	1.00	76.79
ATOM	2134	CZ	TYR	A1055	51.647	71.382	36.644	1.00	76.79
ATOM	2135	OH	TYR	A1055	50.677	70.559	36.119	1.00	76.79
ATOM	2138	N	ARG	A1056	55.598	70.299	38.398	1.00	28.98
ATOM	2139	CA	ARG	A1056	55.836	69.092	37.633	1.00	28.98
ATOM	2140	C	ARG	A1056	54.472	68.506	37.281	1.00	28.98
ATOM	2141	O	ARG	A1056	53.443	68.997	37.844	1.00	28.98
ATOM	2142	CB	ARG	A1056	56.540	68.057	38.504	1.00	43.74
ATOM	2143	CG	ARG	A1056	57.930	68.420	39.046	1.00	43.74
ATOM	2144	CD	ARG	A1056	58.890	68.928	37.990	1.00	43.74
ATOM	2145	NE	ARG	A1056	59.420	70.184	38.476	1.00	43.74
ATOM	2146	CZ	ARG	A1056	60.710	70.421	38.632	1.00	43.74
ATOM	2147	NH1	ARG	A1056	61.589	69.481	38.326	1.00	43.74
ATOM	2148	NH2	ARG	A1056	61.113	71.570	39.153	1.00	43.74
ATOM	2155	N	LEU	A1057	54.457	67.425	36.423	1.00	3.73
ATOM	2156	CA	LEU	A1057	53.199	66.719	36.037	1.00	3.73
ATOM	2157	C	LEU	A1057	52.455	66.273	37.247	1.00	3.73
ATOM	2158	O	LEU	A1057	53.013	65.940	38.293	1.00	3.73
ATOM	2159	CB	LEU	A1057	53.453	65.540	35.129	1.00	53.30
ATOM	2160	CG	LEU	A1057	53.594	65.965	33.659	1.00	53.30

FIG. 6EE

ATOM	2161	CD1	LEU	A1057	54.129	64.770	32.869	1.00	53.30
ATOM	2162	CD2	LEU	A1057	52.271	66.541	33.071	1.00	53.30
ATOM	2164	N	GLU	A1058	51.138	66.322	37.070	1.00	13.17
ATOM	2165	CA	GLU	A1058	50.076	65.947	38.013	1.00	13.17
ATOM	2166	C	GLU	A1058	50.122	64.399	38.274	1.00	13.17
ATOM	2167	O	GLU	A1058	50.140	63.602	37.310	1.00	13.17
ATOM	2168	CB	GLU	A1058	48.779	66.341	37.327	1.00	48.21
ATOM	2169	CG	GLU	A1058	48.686	65.807	35.864	1.00	48.21
ATOM	2170	CD	GLU	A1058	49.433	66.661	34.827	1.00	48.21
ATOM	2171	OE1	GLU	A1058	50.080	67.619	35.269	1.00	48.21
ATOM	2172	OE2	GLU	A1058	49.379	66.410	33.589	1.00	48.21
ATOM	2174	N	LYS	A1059	50.163	63.947	39.531	1.00	35.98
ATOM	2175	CA	LYS	A1059	50.196	62.496	39.689	1.00	35.98
ATOM	2176	C	LYS	A1059	49.010	62.039	38.876	1.00	35.98
ATOM	2177	O	LYS	A1059	47.980	62.696	38.847	1.00	35.98
ATOM	2178	CB	LYS	A1059	50.046	62.040	41.118	1.00	48.90
ATOM	2179	CG	LYS	A1059	50.101	60.540	41.194	1.00	48.90
ATOM	2180	CD	LYS	A1059	50.190	60.048	42.616	1.00	48.90
ATOM	2181	CE	LYS	A1059	48.873	59.367	43.057	1.00	48.90
ATOM	2182	NZ	LYS	A1059	48.940	57.857	43.104	1.00	48.90
ATOM	2187	N	PRO	A1060	49.129	60.936	38.161	1.00	50.25
ATOM	2188	CA	PRO	A1060	47.931	60.601	37.405	1.00	50.25
ATOM	2189	C	PRO	A1060	46.928	59.608	37.964	1.00	50.25
ATOM	2190	O	PRO	A1060	47.176	58.424	37.967	1.00	50.25
ATOM	2191	CB	PRO	A1060	48.504	60.174	36.084	1.00	21.32
ATOM	2192	CG	PRO	A1060	50.037	59.963	36.356	1.00	21.32
ATOM	2193	CD	PRO	A1060	50.246	60.058	37.817	1.00	21.32
ATOM	2194	N	LEU	A1061	45.772	60.120	38.395	1.00	35.93
ATOM	2195	CA	LEU	A1061	44.633	59.371	38.985	1.00	35.93
ATOM	2196	C	LEU	A1061	44.746	57.870	39.239	1.00	35.93
ATOM	2197	O	LEU	A1061	44.731	57.415	40.396	1.00	35.93
ATOM	2198	CB	LEU	A1061	43.368	59.617	38.155	1.00	74.38
ATOM	2199	CG	LEU	A1061	43.355	59.574	36.617	1.00	74.38
ATOM	2200	CD1	LEU	A1061	44.689	59.971	35.997	1.00	74.38
ATOM	2201	CD2	LEU	A1061	42.942	58.174	36.185	1.00	74.38
ATOM	2203	N	ASN	A1062	44.864	57.145	38.117	1.00	56.10
ATOM	2204	CA	ASN	A1062	44.988	55.689	37.947	1.00	56.10
ATOM	2205	C	ASN	A1062	46.399	55.281	38.291	1.00	56.10
ATOM	2206	O	ASN	A1062	46.855	54.240	37.822	1.00	56.10
ATOM	2207	CB	ASN	A1062	44.865	55.366	36.477	1.00	38.56
ATOM	2208	CG	ASN	A1062	46.002	56.035	35.686	1.00	38.56
ATOM	2209	OD1	ASN	A1062	46.683	56.890	36.256	1.00	38.56
ATOM	2210	ND2	ASN	A1062	46.216	55.673	34.397	1.00	38.56
ATOM	2214	N	CYS	A1063	47.109	56.092	39.065	1.00	99.97
ATOM	2215	CA	CYS	A1063	48.503	55.791	39.376	1.00	99.97
ATOM	2216	C	CYS	A1063	48.861	55.613	40.829	1.00	99.97
ATOM	2217	O	CYS	A1063	48.362	56.299	41.699	1.00	99.97
ATOM	2218	CB	CYS	A1063	49.398	56.891	38.827	1.00	81.22
ATOM	2219	SG	CYS	A1063	50.449	56.431	37.527	1.00	81.22
ATOM	2221	N	ASP	A1064	49.770	54.691	41.070	1.00	40.11
ATOM	2222	CA	ASP	A1064	50.260	54.424	42.405	1.00	40.11
ATOM	2223	C	ASP	A1064	51.472	55.243	42.813	1.00	40.11
ATOM	2224	O	ASP	A1064	52.454	55.285	42.109	1.00	40.11
ATOM	2225	CB	ASP	A1064	50.623	52.961	42.560	1.00	60.57
ATOM	2226	CG	ASP	A1064	50.760	52.580	43.992	1.00	60.57
ATOM	2227	OD1	ASP	A1064	50.671	53.492	44.844	1.00	60.57
ATOM	2228	OD2	ASP	A1064	50.941	51.391	44.292	1.00	60.57

FIG. 6FF

ATOM	2230	N	ASP	A1065	51.409	55.855	43.980	1.00	46.39
ATOM	2231	CA	ASP	A1065	52.499	56.662	44.508	1.00	46.39
ATOM	2232	C	ASP	A1065	53.884	56.043	44.229	1.00	46.39
ATOM	2233	O	ASP	A1065	54.869	56.717	44.124	1.00	46.39
ATOM	2234	CB	ASP	A1065	52.299	56.875	46.021	1.00	75.00
ATOM	2235	CG	ASP	A1065	51.156	57.855	46.357	1.00	75.00
ATOM	2236	OD1	ASP	A1065	50.426	58.300	45.452	1.00	75.00
ATOM	2237	OD2	ASP	A1065	50.988	58.179	47.550	1.00	75.00
ATOM	2239	N	GLU	A1066	53.951	54.742	44.107	1.00	29.06
ATOM	2240	CA	GLU	A1066	55.205	54.101	43.803	1.00	29.06
ATOM	2241	C	GLU	A1066	55.543	54.513	42.403	1.00	29.06
ATOM	2242	O	GLU	A1066	56.559	55.189	42.220	1.00	29.06
ATOM	2243	CB	GLU	A1066	55.109	52.567	43.888	1.00	46.46
ATOM	2244	CG	GLU	A1066	56.488	51.877	43.895	1.00	46.46
ATOM	2245	CD	GLU	A1066	56.612	50.697	44.880	1.00	46.46
ATOM	2246	OE1	GLU	A1066	55.711	50.554	45.759	1.00	46.46
ATOM	2247	OE2	GLU	A1066	57.616	49.923	44.765	1.00	46.46
ATOM	2249	N	VAL	A1067	54.727	54.154	41.416	1.00	32.03
ATOM	2250	CA	VAL	A1067	55.023	54.533	40.036	1.00	32.03
ATOM	2251	C	VAL	A1067	55.293	56.054	39.731	1.00	32.03
ATOM	2252	O	VAL	A1067	56.029	56.405	38.812	1.00	32.03
ATOM	2253	CB	VAL	A1067	53.885	54.021	39.107	1.00	15.97
ATOM	2254	CG1	VAL	A1067	53.965	54.642	37.618	1.00	15.97
ATOM	2255	CG2	VAL	A1067	53.929	52.448	39.087	1.00	15.97
ATOM	2257	N	TYR	A1068	54.738	56.973	40.480	1.00	40.19
ATOM	2258	CA	TYR	A1068	55.001	58.328	40.091	1.00	40.19
ATOM	2259	C	TYR	A1068	56.057	58.982	40.941	1.00	40.19
ATOM	2260	O	TYR	A1068	56.899	59.755	40.422	1.00	40.19
ATOM	2261	CB	TYR	A1068	53.684	59.082	40.070	1.00	3.92
ATOM	2262	CG	TYR	A1068	53.658	60.503	40.344	1.00	3.92
ATOM	2263	CD1	TYR	A1068	53.484	61.369	39.326	1.00	3.92
ATOM	2264	CD2	TYR	A1068	53.650	60.958	41.607	1.00	3.92
ATOM	2265	CE1	TYR	A1068	53.296	62.732	39.530	1.00	3.92
ATOM	2266	CE2	TYR	A1068	53.473	62.266	41.862	1.00	3.92
ATOM	2267	CZ	TYR	A1068	53.311	63.163	40.812	1.00	3.92
ATOM	2268	OH	TYR	A1068	53.384	64.523	41.015	1.00	3.92
ATOM	2271	N	ASP	A1069	55.999	58.711	42.242	1.00	34.55
ATOM	2272	CA	ASP	A1069	57.036	59.211	43.139	1.00	34.55
ATOM	2273	C	ASP	A1069	58.139	58.257	42.721	1.00	34.55
ATOM	2274	O	ASP	A1069	58.415	57.326	43.454	1.00	34.55
ATOM	2275	CB	ASP	A1069	56.639	58.964	44.588	1.00	80.97
ATOM	2276	CG	ASP	A1069	57.819	58.905	45.514	1.00	80.97
ATOM	2277	OD1	ASP	A1069	58.968	59.094	45.061	1.00	80.97
ATOM	2278	OD2	ASP	A1069	57.591	58.673	46.714	1.00	80.97
ATOM	2280	N	LEU	A1070	58.667	58.506	41.503	1.00	4.63
ATOM	2281	CA	LEU	A1070	59.682	57.806	40.729	1.00	4.63
ATOM	2282	C	LEU	A1070	59.701	58.504	39.408	1.00	4.63
ATOM	2283	O	LEU	A1070	60.763	58.899	38.932	1.00	4.63
ATOM	2284	CB	LEU	A1070	59.389	56.337	40.348	1.00	35.45
ATOM	2285	CG	LEU	A1070	60.432	56.018	39.208	1.00	35.45
ATOM	2286	CD1	LEU	A1070	61.722	55.660	39.890	1.00	35.45
ATOM	2287	CD2	LEU	A1070	60.081	54.914	38.223	1.00	35.45
ATOM	2289	N	MET	A1071	58.577	58.594	38.714	1.00	33.43
ATOM	2290	CA	MET	A1071	58.662	59.377	37.490	1.00	33.43
ATOM	2291	C	MET	A1071	59.072	60.795	37.999	1.00	33.43
ATOM	2292	O	MET	A1071	59.717	61.547	37.301	1.00	33.43
ATOM	2293	CB	MET	A1071	57.328	59.425	36.716	1.00	46.26

FIG. 6GG

ATOM	2294	CG	MET	A1071	56.293	60.425	37.126	1.00	46.26
ATOM	2295	SD	MET	A1071	54.669	59.634	37.210	1.00	46.26
ATOM	2296	CE	MET	A1071	54.450	58.978	35.595	1.00	46.26
ATOM	2298	N	ARG	A1072	58.729	61.126	39.238	1.00	27.25
ATOM	2299	CA	ARG	A1072	59.114	62.389	39.800	1.00	27.25
ATOM	2300	C	ARG	A1072	60.612	62.482	40.123	1.00	27.25
ATOM	2301	O	ARG	A1072	61.232	63.557	40.039	1.00	27.25
ATOM	2302	CB	ARG	A1072	58.293	62.660	41.064	1.00	100.00
ATOM	2303	CG	ARG	A1072	56.890	63.206	40.805	1.00	100.00
ATOM	2304	CD	ARG	A1072	56.900	64.723	40.605	1.00	100.00
ATOM	2305	NE	ARG	A1072	57.085	65.438	41.861	1.00	100.00
ATOM	2306	CZ	ARG	A1072	56.517	66.600	42.150	1.00	100.00
ATOM	2307	NH1	ARG	A1072	55.722	67.184	41.271	1.00	100.00
ATOM	2308	NH2	ARG	A1072	56.749	67.178	43.315	1.00	100.00
ATOM	2315	N	GLN	A1073	61.212	61.376	40.533	1.00	63.04
ATOM	2316	CA	GLN	A1073	62.625	61.439	40.836	1.00	63.04
ATOM	2317	C	GLN	A1073	63.329	61.922	39.571	1.00	63.04
ATOM	2318	O	GLN	A1073	64.270	62.702	39.623	1.00	63.04
ATOM	2319	CB	GLN	A1073	63.152	60.060	41.233	1.00	85.05
ATOM	2320	CG	GLN	A1073	62.417	59.384	42.387	1.00	85.05
ATOM	2321	CD	GLN	A1073	63.134	58.127	42.896	1.00	85.05
ATOM	2322	OE1	GLN	A1073	62.615	57.410	43.752	1.00	85.05
ATOM	2323	NE2	GLN	A1073	64.322	57.859	42.364	1.00	85.05
ATOM	2327	N	CYS	A1074	62.838	61.488	38.421	1.00	37.06
ATOM	2328	CA	CYS	A1074	63.456	61.841	37.163	1.00	37.06
ATOM	2329	C	CYS	A1074	63.305	63.280	36.845	1.00	37.06
ATOM	2330	O	CYS	A1074	63.613	63.703	35.747	1.00	37.06
ATOM	2331	CB	CYS	A1074	62.838	61.039	36.021	1.00	55.92
ATOM	2332	SG	CYS	A1074	62.574	59.373	36.414	1.00	55.92
ATOM	2334	N	TRP	A1075	62.780	64.030	37.793	1.00	54.40
ATOM	2335	CA	TRP	A1075	62.549	65.443	37.559	1.00	54.40
ATOM	2336	C	TRP	A1075	63.051	66.360	38.693	1.00	54.40
ATOM	2337	O	TRP	A1075	62.683	67.533	38.757	1.00	54.40
ATOM	2338	CB	TRP	A1075	61.055	65.719	37.347	1.00	13.83
ATOM	2339	CG	TRP	A1075	60.306	65.009	36.268	1.00	13.83
ATOM	2340	CD1	TRP	A1075	60.694	64.793	34.985	1.00	13.83
ATOM	2341	CD2	TRP	A1075	58.962	64.566	36.350	1.00	13.83
ATOM	2342	NE1	TRP	A1075	59.683	64.256	34.259	1.00	13.83
ATOM	2343	CE2	TRP	A1075	58.593	64.109	35.078	1.00	13.83
ATOM	2344	CE3	TRP	A1075	58.029	64.518	37.373	1.00	13.83
ATOM	2345	CZ2	TRP	A1075	57.303	63.604	34.801	1.00	13.83
ATOM	2346	CZ3	TRP	A1075	56.751	64.011	37.074	1.00	13.83
ATOM	2347	CH2	TRP	A1075	56.423	63.573	35.814	1.00	13.83
ATOM	2350	N	ARG	A1076	63.867	65.842	39.597	1.00	99.49
ATOM	2351	CA	ARG	A1076	64.354	66.722	40.635	1.00	99.49
ATOM	2352	C	ARG	A1076	64.967	67.872	39.838	1.00	99.49
ATOM	2353	O	ARG	A1076	65.185	67.747	38.637	1.00	99.49
ATOM	2354	CB	ARG	A1076	65.412	66.011	41.484	1.00	96.28
ATOM	2355	CG	ARG	A1076	64.948	64.665	42.026	1.00	96.28
ATOM	2356	CD	ARG	A1076	65.966	64.028	42.968	1.00	96.28
ATOM	2357	NE	ARG	A1076	65.361	63.411	44.155	1.00	96.28
ATOM	2358	CZ	ARG	A1076	65.408	62.110	44.427	1.00	96.28
ATOM	2359	NH1	ARG	A1076	66.029	61.286	43.595	1.00	96.28
ATOM	2360	NH2	ARG	A1076	64.855	61.635	45.538	1.00	96.28
ATOM	2367	N	GLU	A1077	65.200	69.008	40.469	1.00	54.46
ATOM	2368	CA	GLU	A1077	65.824	70.107	39.764	1.00	54.46
ATOM	2369	C	GLU	A1077	67.293	69.771	39.587	1.00	54.46

FIG. 6HH

ATOM	2370	O	GLU	A1077	67.727	69.428	38.509	1.00	54.46
ATOM	2371	CB	GLU	A1077	65.689	71.328	40.555	1.00	10.55
ATOM	2373	N	LYS	A1078	68.050	69.854	40.670	1.00	35.40
ATOM	2374	CA	LYS	A1078	69.476	69.542	40.642	1.00	35.40
ATOM	2375	C	LYS	A1078	69.746	68.345	39.704	1.00	35.40
ATOM	2376	O	LYS	A1078	69.592	67.215	40.099	1.00	35.40
ATOM	2377	CB	LYS	A1078	69.954	69.234	42.058	1.00	95.51
ATOM	2378	CG	LYS	A1078	70.054	70.458	42.936	1.00	95.51
ATOM	2379	CD	LYS	A1078	70.070	70.094	44.414	1.00	95.51
ATOM	2380	CE	LYS	A1078	71.487	70.050	44.990	1.00	95.51
ATOM	2381	NZ	LYS	A1078	71.575	69.341	46.309	1.00	95.51
ATOM	2386	N	PRO	A1079	70.230	68.582	38.481	1.00	54.45
ATOM	2387	CA	PRO	A1079	70.437	67.398	37.643	1.00	54.45
ATOM	2388	C	PRO	A1079	71.172	66.206	38.238	1.00	54.45
ATOM	2389	O	PRO	A1079	70.745	65.097	38.040	1.00	54.45
ATOM	2390	CB	PRO	A1079	71.099	67.958	36.381	1.00	46.70
ATOM	2391	CG	PRO	A1079	70.732	69.385	36.376	1.00	46.70
ATOM	2392	CD	PRO	A1079	70.658	69.817	37.801	1.00	46.70
ATOM	2393	N	TYR	A1080	72.265	66.402	38.968	1.00	100.00
ATOM	2394	CA	TYR	A1080	72.963	65.243	39.542	1.00	100.00
ATOM	2395	C	TYR	A1080	72.128	64.578	40.621	1.00	100.00
ATOM	2396	O	TYR	A1080	72.619	63.747	41.375	1.00	100.00
ATOM	2397	CB	TYR	A1080	74.301	65.630	40.141	1.00	41.54
ATOM	2398	CG	TYR	A1080	74.194	66.859	40.985	1.00	41.54
ATOM	2399	CD1	TYR	A1080	73.912	66.774	42.320	1.00	41.54
ATOM	2400	CD2	TYR	A1080	74.316	68.109	40.422	1.00	41.54
ATOM	2401	CE1	TYR	A1080	73.757	67.883	43.061	1.00	41.54
ATOM	2402	CE2	TYR	A1080	74.158	69.220	41.161	1.00	41.54
ATOM	2403	CZ	TYR	A1080	73.882	69.118	42.480	1.00	41.54
ATOM	2404	OH	TYR	A1080	73.778	70.273	43.233	1.00	41.54
ATOM	2407	N	GLU	A1081	70.870	64.982	40.712	1.00	38.29
ATOM	2408	CA	GLU	A1081	69.948	64.379	41.652	1.00	38.29
ATOM	2409	C	GLU	A1081	69.030	63.423	40.853	1.00	38.29
ATOM	2410	O	GLU	A1081	68.522	62.448	41.398	1.00	38.29
ATOM	2411	CB	GLU	A1081	69.214	65.451	42.451	1.00	37.33
ATOM	2412	CG	GLU	A1081	69.927	65.679	43.797	1.00	37.33
ATOM	2413	CD	GLU	A1081	69.529	66.957	44.542	1.00	37.33
ATOM	2414	OE1	GLU	A1081	70.080	67.203	45.646	1.00	37.33
ATOM	2415	OE2	GLU	A1081	68.676	67.741	44.045	1.00	37.33
ATOM	2417	N	ARG	A1082	68.876	63.690	39.550	1.00	35.27
ATOM	2418	CA	ARG	A1082	68.154	62.803	38.655	1.00	35.27
ATOM	2419	C	ARG	A1082	68.831	61.404	38.883	1.00	35.27
ATOM	2420	O	ARG	A1082	69.932	61.322	39.463	1.00	35.27
ATOM	2421	CB	ARG	A1082	68.336	63.260	37.216	1.00	62.49
ATOM	2422	CG	ARG	A1082	67.202	64.072	36.647	1.00	62.49
ATOM	2423	CD	ARG	A1082	67.299	65.548	36.942	1.00	62.49
ATOM	2424	NE	ARG	A1082	67.442	66.375	35.737	1.00	62.49
ATOM	2425	CZ	ARG	A1082	67.099	67.665	35.661	1.00	62.49
ATOM	2426	NH1	ARG	A1082	66.585	68.293	36.705	1.00	62.49
ATOM	2427	NH2	ARG	A1082	67.317	68.345	34.547	1.00	62.49
ATOM	2434	N	PRO	A1083	68.144	60.280	38.530	1.00	37.62
ATOM	2435	CA	PRO	A1083	68.732	58.945	38.729	1.00	37.62
ATOM	2436	C	PRO	A1083	69.270	58.328	37.461	1.00	37.62
ATOM	2437	O	PRO	A1083	68.905	58.780	36.414	1.00	37.62
ATOM	2438	CB	PRO	A1083	67.541	58.148	39.267	1.00	40.57
ATOM	2439	CG	PRO	A1083	66.294	59.139	39.213	1.00	40.57
ATOM	2440	CD	PRO	A1083	66.721	60.125	38.171	1.00	40.57

FIG. 6II

ATOM	2441	N	SER	A1084	70.157	57.337	37.541	1.00	23.77
ATOM	2442	CA	SER	A1084	70.642	56.597	36.339	1.00	23.77
ATOM	2443	C	SER	A1084	69.465	55.689	35.826	1.00	23.77
ATOM	2444	O	SER	A1084	68.690	55.172	36.633	1.00	23.77
ATOM	2445	CB	SER	A1084	71.772	55.617	36.733	1.00	2.00
ATOM	2446	OG	SER	A1084	71.518	55.019	38.069	1.00	2.00
ATOM	2449	N	PHE	A1085	69.330	55.466	34.520	1.00	44.36
ATOM	2450	CA	PHE	A1085	68.272	54.565	34.032	1.00	44.36
ATOM	2451	C	PHE	A1085	68.458	53.237	34.801	1.00	44.36
ATOM	2452	O	PHE	A1085	67.633	52.852	35.603	1.00	44.36
ATOM	2453	CB	PHE	A1085	68.414	54.399	32.529	1.00	95.75
ATOM	2454	CG	PHE	A1085	68.175	55.669	31.783	1.00	95.75
ATOM	2455	CD1	PHE	A1085	69.088	56.137	30.866	1.00	95.75
ATOM	2456	CD2	PHE	A1085	67.036	56.409	32.022	1.00	95.75
ATOM	2457	CE1	PHE	A1085	68.863	57.321	30.200	1.00	95.75
ATOM	2458	CE2	PHE	A1085	66.807	57.591	31.361	1.00	95.75
ATOM	2459	CZ	PHE	A1085	67.713	58.049	30.452	1.00	95.75
ATOM	2461	N	ALA	A1086	69.541	52.541	34.541	1.00	35.91
ATOM	2462	CA	ALA	A1086	69.894	51.395	35.347	1.00	35.91
ATOM	2463	C	ALA	A1086	69.171	51.316	36.743	1.00	35.91
ATOM	2464	O	ALA	A1086	68.741	50.223	37.179	1.00	35.91
ATOM	2465	CB	ALA	A1086	71.400	51.423	35.580	1.00	44.62
ATOM	2467	N	GLN	A1087	69.081	52.427	37.464	1.00	20.15
ATOM	2468	CA	GLN	A1087	68.394	52.412	38.732	1.00	20.15
ATOM	2469	C	GLN	A1087	66.842	52.338	38.466	1.00	20.15
ATOM	2470	O	GLN	A1087	66.039	51.538	39.059	1.00	20.15
ATOM	2471	CB	GLN	A1087	68.766	53.690	39.501	1.00	19.20
ATOM	2472	CG	GLN	A1087	70.227	53.686	40.069	1.00	19.20
ATOM	2473	CD	GLN	A1087	70.563	54.908	40.926	1.00	19.20
ATOM	2474	OE1	GLN	A1087	70.927	55.939	40.379	1.00	19.20
ATOM	2475	NE2	GLN	A1087	70.473	54.783	42.263	1.00	19.20
ATOM	2479	N	ILE	A1088	66.451	53.197	37.550	1.00	25.82
ATOM	2480	CA	ILE	A1088	65.088	53.310	37.160	1.00	25.82
ATOM	2481	C	ILE	A1088	64.852	51.851	36.847	1.00	25.82
ATOM	2482	O	ILE	A1088	63.966	51.300	37.447	1.00	25.82
ATOM	2483	CB	ILE	A1088	64.921	54.260	35.919	1.00	17.84
ATOM	2484	CG1	ILE	A1088	65.069	55.704	36.340	1.00	17.84
ATOM	2485	CG2	ILE	A1088	63.626	53.984	35.170	1.00	17.84
ATOM	2486	CD1	ILE	A1088	65.738	56.545	35.203	1.00	17.84
ATOM	2488	N	LEU	A1089	65.628	51.205	35.969	1.00	19.62
ATOM	2489	CA	LEU	A1089	65.380	49.747	35.692	1.00	19.62
ATOM	2490	C	LEU	A1089	65.471	48.746	36.793	1.00	19.62
ATOM	2491	O	LEU	A1089	64.899	47.746	36.680	1.00	19.62
ATOM	2492	CB	LEU	A1089	66.155	49.127	34.566	1.00	2.73
ATOM	2493	CG	LEU	A1089	65.363	47.832	33.978	1.00	2.73
ATOM	2494	CD1	LEU	A1089	65.305	47.787	32.425	1.00	2.73
ATOM	2495	CD2	LEU	A1089	66.127	46.642	34.338	1.00	2.73
ATOM	2497	N	VAL	A1090	66.164	48.988	37.866	1.00	15.82
ATOM	2498	CA	VAL	A1090	66.074	47.993	38.898	1.00	15.82
ATOM	2499	C	VAL	A1090	64.931	48.400	39.791	1.00	15.82
ATOM	2500	O	VAL	A1090	64.700	47.776	40.834	1.00	15.82
ATOM	2501	CB	VAL	A1090	67.396	47.811	39.695	1.00	8.61
ATOM	2502	CG1	VAL	A1090	67.259	48.053	41.220	1.00	8.61
ATOM	2503	CG2	VAL	A1090	67.829	46.397	39.452	1.00	8.61
ATOM	2505	N	SER	A1091	64.218	49.451	39.377	1.00	45.24
ATOM	2506	CA	SER	A1091	63.073	50.005	40.110	1.00	45.24
ATOM	2507	C	SER	A1091	61.708	49.486	39.628	1.00	45.24

ATOM	2508	O	SER	A1091	60.764	49.305	40.422	1.00	45.24
ATOM	2509	CB	SER	A1091	63.064	51.511	39.963	1.00	46.04
ATOM	2510	OG	SER	A1091	62.473	52.119	41.083	1.00	46.04
ATOM	2513	N	LEU	A1092	61.582	49.317	38.318	1.00	48.10
ATOM	2514	CA	LEU	A1092	60.336	48.814	37.772	1.00	48.10
ATOM	2515	C	LEU	A1092	60.362	47.286	37.896	1.00	48.10
ATOM	2516	O	LEU	A1092	59.310	46.649	38.093	1.00	48.10
ATOM	2517	CB	LEU	A1092	60.226	49.217	36.335	1.00	20.50
ATOM	2518	CG	LEU	A1092	60.649	50.636	36.171	1.00	20.50
ATOM	2519	CD1	LEU	A1092	61.112	50.957	34.819	1.00	20.50
ATOM	2520	CD2	LEU	A1092	59.492	51.389	36.445	1.00	20.50
ATOM	2522	N	ASN	A1093	61.588	46.721	37.764	1.00	21.90
ATOM	2523	CA	ASN	A1093	61.816	45.284	37.914	1.00	21.90
ATOM	2524	C	ASN	A1093	61.298	44.970	39.321	1.00	21.90
ATOM	2525	O	ASN	A1093	60.506	44.064	39.515	1.00	21.90
ATOM	2526	CB	ASN	A1093	63.301	45.010	37.802	1.00	40.34
ATOM	2527	CG	ASN	A1093	63.756	44.903	36.364	1.00	40.34
ATOM	2528	OD1	ASN	A1093	64.796	44.322	36.103	1.00	40.34
ATOM	2529	ND2	ASN	A1093	62.989	45.468	35.422	1.00	40.34
ATOM	2533	N	ARG	A1094	61.699	45.746	40.314	1.00	34.76
ATOM	2534	CA	ARG	A1094	61.194	45.385	41.611	1.00	34.76
ATOM	2535	C	ARG	A1094	59.685	45.221	41.451	1.00	34.76
ATOM	2536	O	ARG	A1094	59.122	44.320	42.022	1.00	34.76
ATOM	2537	CB	ARG	A1094	61.515	46.451	42.653	1.00	99.74
ATOM	2538	CG	ARG	A1094	61.377	45.969	44.088	1.00	99.74
ATOM	2539	CD	ARG	A1094	59.934	46.037	44.575	1.00	99.74
ATOM	2540	NE	ARG	A1094	59.736	47.099	45.557	1.00	99.74
ATOM	2541	CZ	ARG	A1094	58.550	47.590	45.907	1.00	99.74
ATOM	2542	NH1	ARG	A1094	57.438	47.117	45.357	1.00	99.74
ATOM	2543	NH2	ARG	A1094	58.479	48.565	46.805	1.00	99.74
ATOM	2550	N	MET	A1095	59.045	46.073	40.640	1.00	52.46
ATOM	2551	CA	MET	A1095	57.594	46.029	40.452	1.00	52.46
ATOM	2552	C	MET	A1095	57.136	44.721	39.781	1.00	52.46
ATOM	2553	O	MET	A1095	56.663	43.809	40.435	1.00	52.46
ATOM	2554	CB	MET	A1095	57.151	47.287	39.683	1.00	62.45
ATOM	2555	CG	MET	A1095	57.076	48.578	40.594	1.00	62.45
ATOM	2556	SD	MET	A1095	57.031	50.297	39.847	1.00	62.45
ATOM	2557	CE	MET	A1095	57.509	51.299	41.162	1.00	62.45
ATOM	2559	N	LEU	A1096	57.289	44.666	38.476	1.00	14.04
ATOM	2560	CA	LEU	A1096	57.029	43.531	37.600	1.00	14.04
ATOM	2561	C	LEU	A1096	57.039	42.101	38.255	1.00	14.04
ATOM	2562	O	LEU	A1096	56.575	41.148	37.638	1.00	14.04
ATOM	2563	CB	LEU	A1096	58.046	43.560	36.441	1.00	37.25
ATOM	2564	CG	LEU	A1096	58.047	44.610	35.300	1.00	37.25
ATOM	2565	CD1	LEU	A1096	59.158	44.291	34.269	1.00	37.25
ATOM	2566	CD2	LEU	A1096	56.643	44.684	34.592	1.00	37.25
ATOM	2568	N	GLU	A1097	57.574	41.928	39.450	1.00	42.58
ATOM	2569	CA	GLU	A1097	57.530	40.621	40.048	1.00	42.58
ATOM	2570	C	GLU	A1097	56.651	40.690	41.296	1.00	42.58
ATOM	2571	O	GLU	A1097	57.019	40.286	42.411	1.00	42.58
ATOM	2572	CB	GLU	A1097	58.919	40.136	40.396	1.00	100.00
ATOM	2573	CG	GLU	A1097	59.757	39.901	39.188	1.00	100.00
ATOM	2574	CD	GLU	A1097	60.925	40.839	39.144	1.00	100.00
ATOM	2575	OE1	GLU	A1097	61.083	41.611	40.117	1.00	100.00
ATOM	2576	OE2	GLU	A1097	61.680	40.799	38.147	1.00	100.00
ATOM	2578	N	GLU	A1098	55.454	41.211	41.108	1.00	43.50
ATOM	2579	CA	GLU	A1098	54.540	41.313	42.226	1.00	43.50

FIG. 6KK

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ATOM	2580	C	GLU	A1098	53.112	41.239	41.679	1.00	43.50
ATOM	2581	O	GLU	A1098	52.247	40.533	42.228	1.00	43.50
ATOM	2582	CB	GLU	A1098	54.783	42.639	42.970	1.00	60.12
ATOM	2583	CG	GLU	A1098	56.233	43.014	43.093	1.00	60.12
ATOM	2584	CD	GLU	A1098	56.895	42.498	44.392	1.00	60.12
ATOM	2585	OE1	GLU	A1098	56.253	42.586	45.481	1.00	60.12
ATOM	2586	OE2	GLU	A1098	58.071	42.019	44.331	1.00	60.12
ATOM	2588	N	ARG	A1099	52.896	41.931	40.566	1.00	100.00
ATOM	2589	CA	ARG	A1099	51.564	42.010	40.005	1.00	100.00
ATOM	2590	C	ARG	A1099	50.792	42.471	41.232	1.00	100.00
ATOM	2591	O	ARG	A1099	50.117	41.681	41.899	1.00	100.00
ATOM	2592	CB	ARG	A1099	51.050	40.643	39.530	1.00	69.49
ATOM	2593	CG	ARG	A1099	49.707	40.745	38.761	1.00	69.49
ATOM	2594	CD	ARG	A1099	49.883	40.941	37.244	1.00	69.49
ATOM	2595	NE	ARG	A1099	49.647	42.326	36.812	1.00	69.49
ATOM	2596	CZ	ARG	A1099	49.095	42.672	35.648	1.00	69.49
ATOM	2597	NH1	ARG	A1099	48.705	41.740	34.782	1.00	69.49
ATOM	2598	NH2	ARG	A1099	48.989	43.951	35.322	1.00	69.49
ATOM	2605	N	LYS	A1100	50.957	43.748	41.555	1.00	49.25
ATOM	2606	CA	LYS	A1100	50.308	44.328	42.698	1.00	49.25
ATOM	2607	C	LYS	A1100	49.232	45.070	42.019	1.00	49.25
ATOM	2608	O	LYS	A1100	48.111	45.129	42.502	1.00	49.25
ATOM	2609	CB	LYS	A1100	51.247	45.296	43.419	1.00	99.82
ATOM	2610	CG	LYS	A1100	50.853	45.635	44.859	1.00	99.82
ATOM	2611	CD	LYS	A1100	50.997	44.447	45.815	1.00	99.82
ATOM	2612	CE	LYS	A1100	49.635	43.868	46.212	1.00	99.82
ATOM	2613	NZ	LYS	A1100	49.247	44.148	47.622	1.00	99.82
ATOM	2618	N	THR	A1101	49.603	45.578	40.850	1.00	64.74
ATOM	2619	CA	THR	A1101	48.769	46.370	39.946	1.00	64.74
ATOM	2620	C	THR	A1101	49.030	47.835	40.194	1.00	64.74
ATOM	2621	O	THR	A1101	48.381	48.463	41.014	1.00	64.74
ATOM	2622	CB	THR	A1101	47.282	46.080	40.069	1.00	100.00
ATOM	2623	OG1	THR	A1101	47.083	44.676	40.244	1.00	100.00
ATOM	2624	CG2	THR	A1101	46.581	46.494	38.801	1.00	100.00
ATOM	2627	N	TYR	A1102	50.026	48.346	39.472	1.00	78.61
ATOM	2628	CA	TYR	A1102	50.462	49.715	39.571	1.00	78.61
ATOM	2629	C	TYR	A1102	49.666	50.619	38.672	1.00	78.61
ATOM	2630	O	TYR	A1102	49.438	51.753	39.026	1.00	78.61
ATOM	2631	CB	TYR	A1102	51.960	49.856	39.210	1.00	42.69
ATOM	2632	CG	TYR	A1102	52.910	49.107	40.092	1.00	42.69
ATOM	2633	CD1	TYR	A1102	53.228	47.735	39.812	1.00	42.69
ATOM	2634	CD2	TYR	A1102	53.356	49.663	41.288	1.00	42.69
ATOM	2635	CE1	TYR	A1102	53.926	46.943	40.711	1.00	42.69
ATOM	2636	CE2	TYR	A1102	54.061	48.880	42.207	1.00	42.69
ATOM	2637	CZ	TYR	A1102	54.327	47.512	41.917	1.00	42.69
ATOM	2638	OH	TYR	A1102	54.871	46.698	42.873	1.00	42.69
ATOM	2641	N	VAL	A1103	49.233	50.151	37.513	1.00	100.00
ATOM	2642	CA	VAL	A1103	48.509	51.066	36.650	1.00	100.00
ATOM	2643	C	VAL	A1103	47.068	50.762	36.293	1.00	100.00
ATOM	2644	O	VAL	A1103	46.757	50.368	35.175	1.00	100.00
ATOM	2645	CB	VAL	A1103	49.276	51.326	35.350	1.00	100.00
ATOM	2646	CG1	VAL	A1103	48.590	52.426	34.565	1.00	100.00
ATOM	2647	CG2	VAL	A1103	50.694	51.746	35.661	1.00	100.00
ATOM	2649	N	ASN	A1104	46.191	50.990	37.260	1.00	30.52
ATOM	2650	CA	ASN	A1104	44.768	50.802	37.118	1.00	30.52
ATOM	2651	C	ASN	A1104	44.245	51.216	35.761	1.00	30.52
ATOM	2652	O	ASN	A1104	44.475	52.317	35.289	1.00	30.52

FIG. 6LL

ATOM	2653	CB	ASN	A1104	44.041	51.572	38.171	1.00	63.62
ATOM	2654	CG	ASN	A1104	42.646	51.154	38.272	1.00	63.62
ATOM	2655	OD1	ASN	A1104	41.934	51.137	37.275	1.00	63.62
ATOM	2656	ND2	ASN	A1104	42.224	50.788	39.469	1.00	63.62
ATOM	2660	N	THR	A1105	43.519	50.305	35.135	1.00	45.33
ATOM	2661	CA	THR	A1105	42.978	50.501	33.817	1.00	45.33
ATOM	2662	C	THR	A1105	41.629	49.788	33.751	1.00	45.33
ATOM	2663	O	THR	A1105	40.980	49.726	32.734	1.00	45.33
ATOM	2664	CB	THR	A1105	43.987	49.959	32.817	1.00	46.03
ATOM	2665	OG1	THR	A1105	44.604	48.759	33.328	1.00	46.03
ATOM	2666	CG2	THR	A1105	45.083	50.972	32.633	1.00	46.03
ATOM	2669	N	THR	A1105	41.199	49.243	34.869	1.00	15.59
ATOM	2670	CA	THR	A1106	39.900	48.589	34.956	1.00	15.59
ATOM	2671	C	THR	A1106	38.820	49.661	35.289	1.00	15.59
ATOM	2672	O	THR	A1106	39.072	50.461	36.167	1.00	15.59
ATOM	2673	CB	THR	A1106	39.931	47.514	36.091	1.00	59.09
ATOM	2674	OG1	THR	A1106	39.776	46.205	35.525	1.00	59.09
ATOM	2675	CG2	THR	A1106	38.827	47.743	37.083	1.00	59.09
ATOM	2678	N	LEU	A1107	37.641	49.683	34.662	1.00	27.67
ATOM	2679	CA	LEU	A1107	36.613	50.729	35.028	1.00	27.67
ATOM	2680	C	LEU	A1107	35.966	50.401	36.392	1.00	27.67
ATOM	2681	O	LEU	A1107	34.939	49.735	36.477	1.00	27.67
ATOM	2682	CB	LEU	A1107	35.491	50.874	33.967	1.00	39.85
ATOM	2683	CG	LEU	A1107	35.834	50.768	32.492	1.00	39.85
ATOM	2684	CD1	LEU	A1107	34.611	50.486	31.731	1.00	39.85
ATOM	2685	CD2	LEU	A1107	36.500	51.981	31.985	1.00	39.85
ATOM	2687	N	TYR	A1108	36.576	50.816	37.480	1.00	99.39
ATOM	2688	CA	TYR	A1108	35.969	50.482	38.748	1.00	99.39
ATOM	2689	C	TYR	A1108	34.685	51.305	38.878	1.00	99.39
ATOM	2690	O	TYR	A1108	33.900	51.097	39.806	1.00	99.39
ATOM	2691	CB	TYR	A1108	36.973	50.749	39.872	1.00	100.00
ATOM	2692	CG	TYR	A1108	38.383	50.249	39.513	1.00	100.00
ATOM	2693	CD1	TYR	A1108	39.286	51.419	39.214	1.00	100.00
ATOM	2694	CD2	TYR	A1108	38.945	49.421	40.644	1.00	100.00
ATOM	2696	N	GLU	A1109	34.486	52.198	37.899	1.00	100.00
ATOM	2697	CA	GLU	A1109	33.341	53.116	37.779	1.00	100.00
ATOM	2698	C	GLU	A1109	33.875	54.536	37.598	1.00	100.00
ATOM	2699	O	GLU	A1109	34.957	54.846	38.095	1.00	100.00
ATOM	2700	CB	GLU	A1109	32.454	53.065	39.001	1.00	76.82
ATOM	2702	N	LYS	A1110	33.104	55.390	36.914	1.00	100.00
ATOM	2703	CA	LYS	A1110	33.486	56.779	36.626	1.00	100.00
ATOM	2704	C	LYS	A1110	34.891	56.830	36.038	1.00	100.00
ATOM	2705	O	LYS	A1110	35.858	56.673	36.763	1.00	100.00
ATOM	2706	CB	LYS	A1110	33.430	57.631	37.900	1.00	99.15
ATOM	2707	CG	LYS	A1110	34.009	56.977	39.152	1.00	99.15
ATOM	2708	CD	LYS	A1110	34.718	57.970	40.052	1.00	99.15
ATOM	2709	CE	LYS	A1110	34.246	57.852	41.490	1.00	99.15
ATOM	2710	NZ	LYS	A1110	33.479	59.054	41.919	1.00	99.15
ATOM	2715	N	PHE	A1111	35.030	57.055	34.737	1.00	100.00
ATOM	2716	CA	PHE	A1111	36.373	57.068	34.186	1.00	100.00
ATOM	2717	C	PHE	A1111	36.824	58.244	33.333	1.00	100.00
ATOM	2718	O	PHE	A1111	36.116	58.763	32.487	1.00	100.00
ATOM	2719	CB	PHE	A1111	36.685	55.747	33.449	1.00	61.16
ATOM	2720	CG	PHE	A1111	38.144	55.601	33.081	1.00	61.16
ATOM	2721	CD1	PHE	A1111	39.101	55.397	34.055	1.00	61.16
ATOM	2722	CD2	PHE	A1111	38.575	55.820	31.785	1.00	61.16
ATOM	2723	CE1	PHE	A1111	40.448	55.431	33.736	1.00	61.16

FIG. 6MM

ATOM	2724	CE2	PHE	A1111	39.917	55.853	31.485	1.00	61.16	
ATOM	2725	CZ	PHE	A1111	40.845	55.664	32.451	1.00	61.16	
ATOM	2727	N	THR	A1112	38.080	58.579	33.586	1.00	54.03	
ATOM	2728	CA	THR	A1112	38.875	59.664	33.030	1.00	54.03	
ATOM	2729	C	THR	A1112	39.433	59.610	31.628	1.00	54.03	
ATOM	2730	O	THR	A1112	38.693	59.607	30.694	1.00	54.03	
ATOM	2731	CB	THR	A1112	40.029	59.942	34.007	1.00	100.00	
ATOM	2732	OG1	THR	A1112	41.181	59.195	33.618	1.00	100.00	
ATOM	2733	CG2	THR	A1112	39.637	59.498	35.430	1.00	100.00	
ATOM	2736	N	TYR	A1113	40.750	59.639	31.504	1.00	39.45	
ATOM	2737	CA	TYR	A1113	41.514	59.623	30.240	1.00	39.45	
ATOM	2738	C	TYR	A1113	42.391	60.886	30.057	1.00	39.45	
ATOM	2739	O	TYR	A1113	42.658	61.611	30.980	1.00	39.45	
ATOM	2740	CB	TYR	A1113	40.661	59.461	29.000	1.00	60.42	
ATOM	2741	CG	TYR	A1113	40.682	58.097	28.373	1.00	60.42	
ATOM	2742	CD1	TYR	A1113	40.003	57.867	27.193	1.00	60.42	
ATOM	2743	CD2	TYR	A1113	41.168	56.982	29.056	1.00	60.42	
ATOM	2744	CE1	TYR	A1113	39.776	56.585	26.720	1.00	60.42	
ATOM	2745	CE2	TYR	A1113	40.938	55.670	28.577	1.00	60.42	
ATOM	2746	CZ	TYR	A1113	40.231	55.511	27.413	1.00	60.42	
ATOM	2747	OH	TYR	A1113	39.943	54.290	26.912	1.00	60.42	
ATOM	2750	N	ALA	A1114	42.852	61.153	28.847	1.00	100.00	
ATOM	2751	CA	ALA	A1114	43.759	62.268	28.741	1.00	100.00	
ATOM	2752	C	ALA	A1114	44.080	62.762	27.312	1.00	100.00	
ATOM	2753	O	ALA	A1114	44.093	63.971	27.052	1.00	100.00	
ATOM	2754	CB	ALA	A1114	45.049	61.857	29.500	1.00	34.32	
ATOM	2756	N	GLY	A1115	44.317	61.803	26.410	1.00	68.47	
ATOM	2757	CA	GLY	A1115	44.683	62.024	24.996	1.00	68.47	
ATOM	2758	C	GLY	A1115	44.399	63.213	24.093	1.00	68.47	
ATOM	2759	O	GLY	A1115	45.017	63.303	23.036	1.00	68.47	
ATOM	2761	N	ILE	A1116	43.470	64.088	24.487	1.00	100.00	
ATOM	2762	CA	ILE	A1116	43.066	65.299	23.739	1.00	100.00	
ATOM	2763	C	ILE	A1116	41.700	65.193	23.039	1.00	100.00	
ATOM	2764	O	ILE	A1116	41.049	64.140	23.163	1.00	100.00	
ATOM	2765	CB	ILE	A1116	44.141	65.709	22.727	1.00	87.32	
ATOM	2766	OXT	ILE	A1116	41.280	66.178	22.385	1.00	87.32	
TER										
HETATM	1	C1	INH	I	1	58.113	50.247	12.231	0.00	0.00
HETATM	2	N2	INH	I	1	57.524	51.444	12.202	0.00	0.00
HETATM	3	C3	INH	I	1	58.303	52.541	12.107	0.00	0.00
HETATM	4	C4	INH	I	1	59.686	52.462	12.036	0.00	0.00
HETATM	5	C5	INH	I	1	60.234	51.117	12.080	0.00	0.00
HETATM	6	N6	INH	I	1	59.434	50.040	12.174	0.00	0.00
HETATM	8	N8	INH	I	1	57.877	53.857	12.079	0.00	0.00
HETATM	9	C9	INH	I	1	59.057	54.550	11.988	0.00	0.00
HETATM	10	C10	INH	I	1	60.219	53.760	11.953	0.00	0.00
HETATM	12	C13	INH	I	1	61.633	54.217	11.871	0.00	0.00
HETATM	13	N15	INH	I	1	61.632	50.906	12.042	0.00	0.00
HETATM	14	C16	INH	I	1	56.477	54.327	12.146	0.00	0.00
HETATM	15	C17	INH	I	1	56.258	55.192	13.391	0.00	0.00
HETATM	16	C18	INH	I	1	54.809	55.688	13.471	0.00	0.00
HETATM	17	C19	INH	I	1	54.371	56.477	12.214	0.00	0.00
HETATM	18	C20	INH	I	1	54.670	55.630	10.955	0.00	0.00
HETATM	19	C21	INH	I	1	56.121	55.136	10.897	0.00	0.00
HETATM	28	N30	INH	I	1	52.949	56.902	12.268	0.00	0.00
HETATM	29	C32	INH	I	1	51.997	55.774	12.311	0.00	0.00
HETATM	30	C33	INH	I	1	50.531	56.215	12.400	0.00	0.00

FIG. 6NN

Kinase catalytic domain structure walkthrough - insulin receptor kinase

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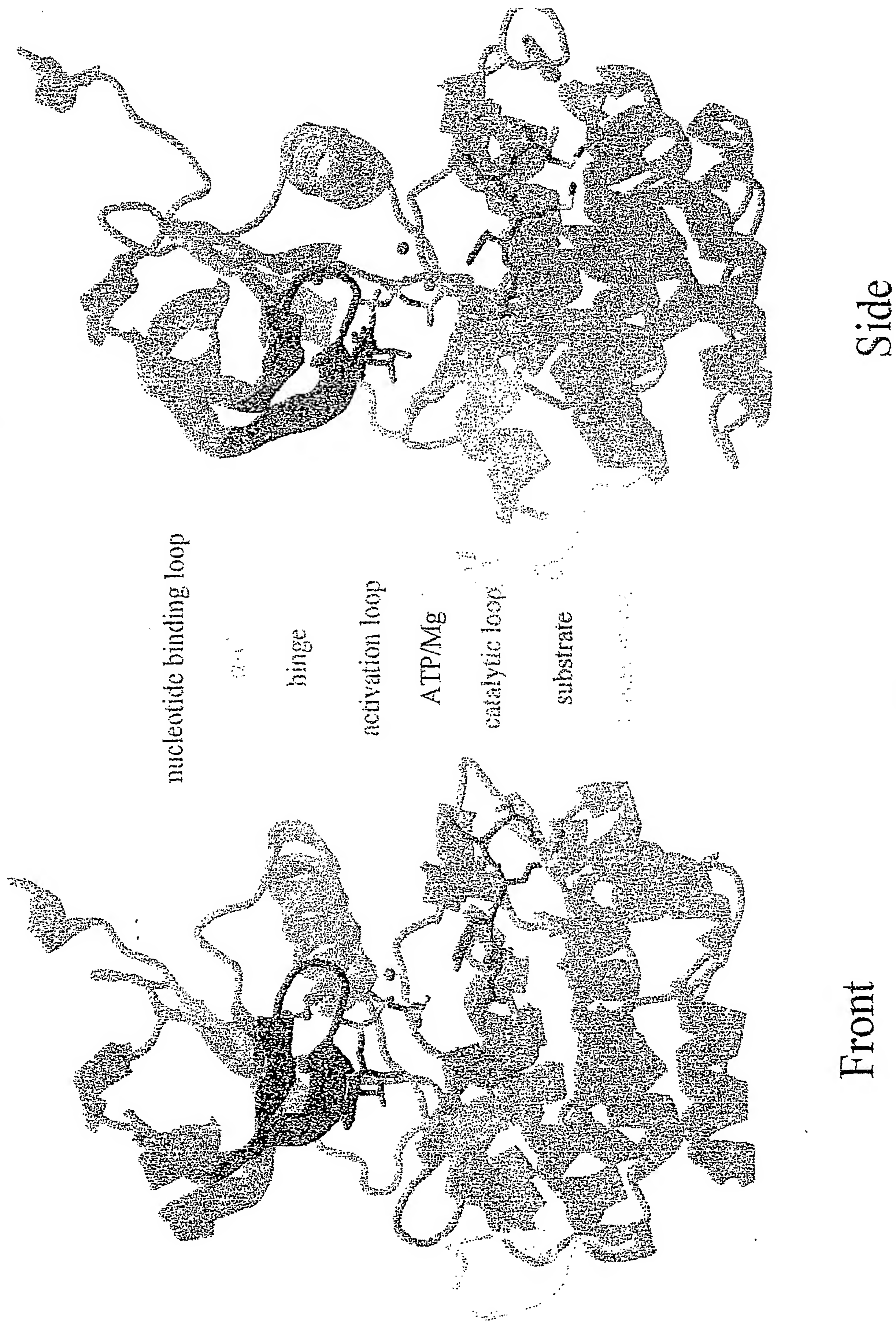


FIG. 7

Inhibitor I structural elements

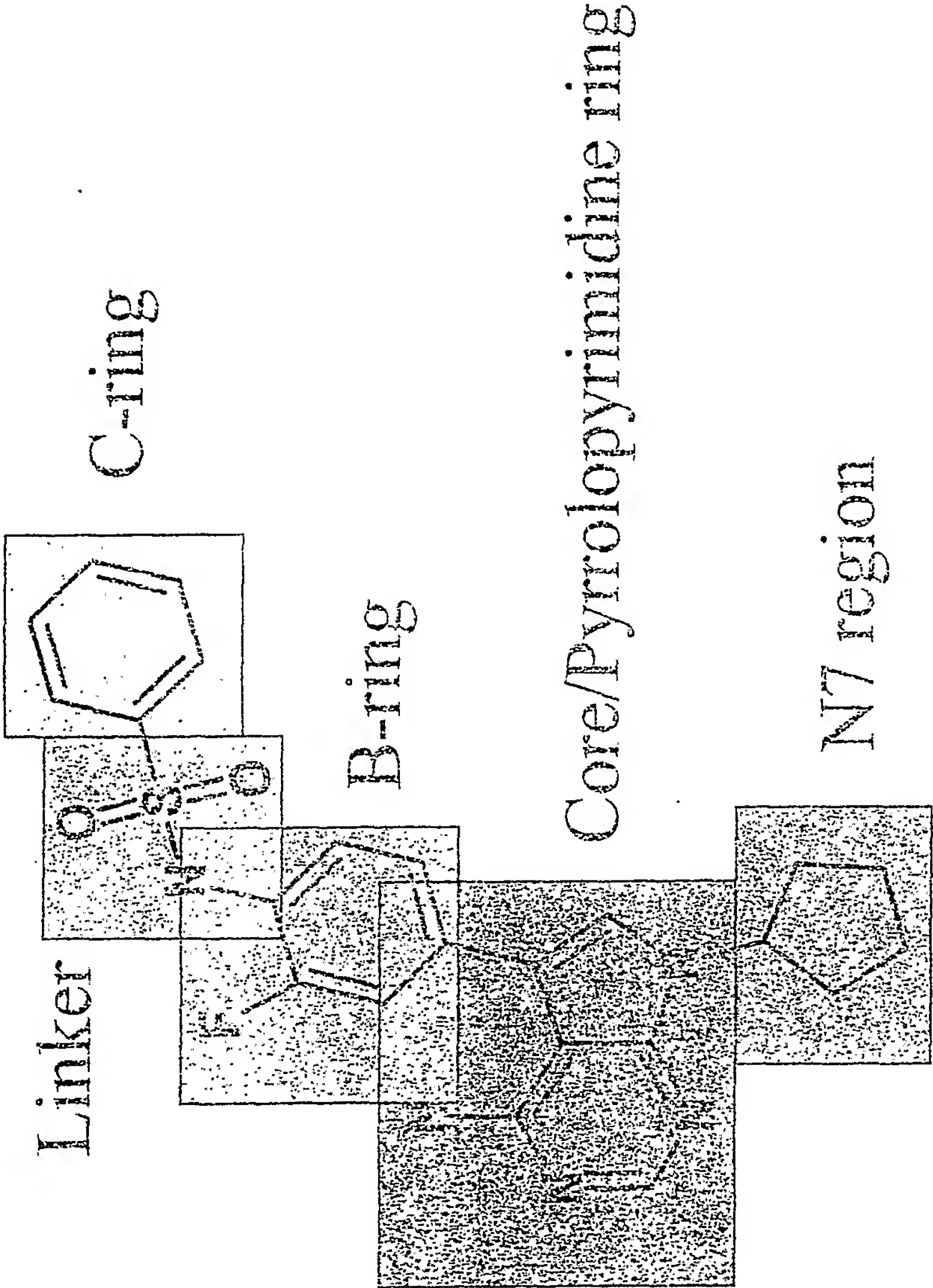
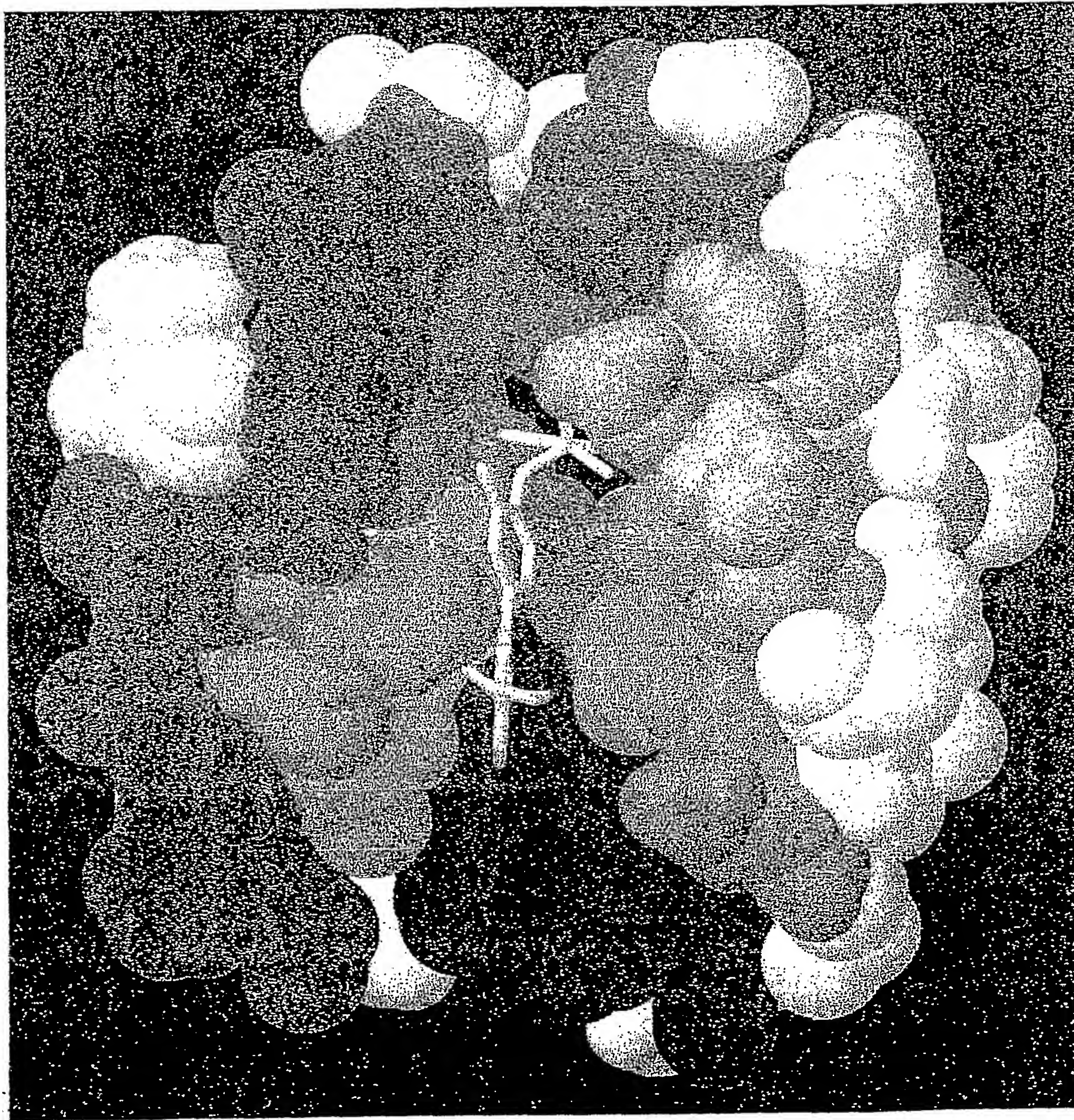


FIG. 8

BSF421386 binding region



hinge
 purine core
 extended sugar
 γ-phosphate
 nucleotide binding
 early activation loop
 catalytic lysine
 distal hydrophobic
 miscellaneous

FIG. 9

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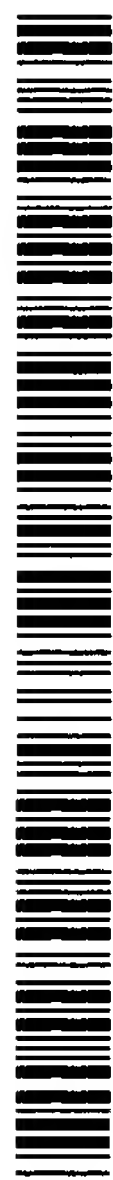
— with international search report

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For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: METHOD OF IDENTIFYING INHIBITORS OF TIE-2

(57) Abstract: The present invention relates to polypeptides which comprise the ligand binding domain of Tie-2, crystalline forms of these polypeptides and the use of these crystalline forms to determine the three dimensional structure of the catalytic domain of Tie-2. The invention also relates to the use of the three dimensional structure of the Tie-2 catalytic domain both alone, or in complex with inhibitors, in methods of designing and/or identifying potential inhibitors of Tie-2 activity, for example, compounds which inhibit the binding of a native substrate to the Tie-2 catalytic domain.



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INTERNATIONAL SEARCH REPORT

International Application No

PCT/US 01/08853

A. CLASSIFICATION OF SUBJECT MATTER

IPC 7 C07K14/71 G01N33/68 A61P35/00

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

IPC 7 C07K G01N

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, WPI Data, PAJ, BIOSIS, MEDLINE, CHEM ABS Data, SEQUENCE SEARCH

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	WO 98 07835 A (SCHLESSINGER JOSEPH ; LIANG CONGXIN (US); SUGEN INC (US); TANG PENG) 26 February 1998 (1998-02-26) claims; examples	1-3, 87, 88
A	WO 98 41525 A (KNOLL AG ; CALDERWOOD DAVID JOHN (GB); JOHNSTON DAVID NORMAN (GB);) 24 September 1998 (1998-09-24) claims; examples	1, 7



Further documents are listed in the continuation of box C.



Patent family members are listed in annex.

* Special categories of cited documents :

- *A* document defining the general state of the art which is not considered to be of particular relevance
- *E* earlier document but published on or after the international filing date
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- *X* document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
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- *&* document member of the same patent family

Date of the actual completion of the international search

5 February 2002

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Fuhr, C

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

Continuation of Box I.2

Claims Nos.: 21-86

Present claims 21-75 relate to a method defined by reference to a desirable characteristic, namely a method for finding a compound which fits into a catalytic domain by use of the atomic coordinates of a crystal of the catalytic domain, and the compounds identified therewith.

The claims cover all methods and compounds having this characteristic, whereas the application provides no support within the meaning of Article 6 PCT and/or no disclosure within the meaning of Article 5 PCT for such methods and compounds. In the present case, the claims so lack support, and the application so lacks disclosure, that a meaningful search over the whole of the claimed scope is impossible. Independent of the above reasoning, the claims also lack clarity (Article 6 PCT). An attempt is made to define the method and compounds by reference to a result to be achieved. Again, this lack of clarity in the present case is such as to render a meaningful search over the whole of the claimed scope impossible. Consequently, the no search has been carried out for those claims.

Present claims 76-86 relate to a method defined by reference to a desirable characteristic or property, namely a method of treatment of a tie-2 related condition by administration of a compound found with above mentioned method.

The claims cover all methods having this characteristic or property, whereas the application provides no support within the meaning of Article 6 PCT and/or no disclosure within the meaning of Article 5 PCT for such methods. In the present case, the claims so lack support, and the application so lacks disclosure, that a meaningful search over the whole of the claimed scope is impossible. Independent of the above reasoning, the claims also lack clarity (Article 6 PCT). An attempt is made to define the method by reference to a result to be achieved. Again, this lack of clarity in the present case is such as to render a meaningful search over the whole of the claimed scope impossible. Consequently, no search has been carried out for those claims.

The applicant's attention is drawn to the fact that claims, or parts of claims, relating to inventions in respect of which no international search report has been established need not be the subject of an international preliminary examination (Rule 66.1(e) PCT). The applicant is advised that the EPO policy when acting as an International Preliminary Examining Authority is normally not to carry out a preliminary examination on matter which has not been searched. This is the case irrespective of whether or not the claims are amended following receipt of the search report or during any Chapter II procedure.

INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No

PCT/US 01/08853

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
WO 9807835	A	26-02-1998	US 5942428 A
			AU 733890 B2
			AU 4160397 A
			EP 0931152 A2
			JP 2001514484 T
			WO 9807835 A2
WO 9841525	A	24-09-1998	AU 6829398 A
			BG 103785 A
			BR 9808281 A
			CN 1259950 T
			WO 9841525 A1
			EP 0970084 A1
			HU 0001507 A2
			JP 2001516353 T
			NO 994509 A
			PL 335685 A1
			SK 125999 A3
			TR 9902301 T2
			US 6001839 A